# Monday Morning, October 30, 2017

## 2D Materials Focus Topic
## Room 15 - Session 2D+EM+MI+MN-MoM

### Properties of 2D Materials including Electronic, Magnetic, Mechanical, Optical, and Thermal Properties

**Moderator:** Andrey Turchanin, Friedrich Schiller University Jena, Germany

8:20am **2D+EM+MI+MN-MoM-1 Spontaneous Mechanical Buckling in Two-Dimensional Materials: A Power Source for Ambient Vibration Energy Harvesters***, **Paul Thibado**, P Kumar, S Singh,* University of Arkansas

Internet-of-Things (IoT) is projected to become a multi-trillion-dollar market, but most applications cannot afford replacing batteries on such a large scale, driving the need for battery alternatives.

We recently discovered that freestanding graphene membranes are in perpetual motion when held at room temperature [1-3]. Surprisingly, the random up-down motion of the membrane does not follow classical Brownian motion, but instead is super-diffusive at short times and sub-diffusive at long times. Furthermore, the velocity probability distribution function is non-Gaussian and follows the heavy-tailed Cauchy-Lorentz distribution, consistent with Levy flights.

Molecular dynamics simulations reveal that mechanical buckling is spontaneously occurring, and that this is the mechanism responsible for the anomalous movement. Bucking in this system occurs when the local material suddenly flips from concave to convex.

The higher kinetic energy associated with this motion is derived from the surrounding thermal waste heat, and it may be converted into an electrical current and used as the active component of small power generators known as ambient vibration energy harvesters.

References:

[1] P. Xu, M. Neek-Amal, S.D. Barber, J.K. Schoelz, M.L. Ackerman, P.M. Thibado, A. Sadeghi, and F.M. Peeters, Nature Comm. **5**, 3720 (2014).

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[3] M.L. Ackerman, P. Kumar, M. Neek-Amal, P.M. Thibado, F.M. Peeters, and S.P. Singh, Phys., Rev. Lett. **117**, 126801 (2016).

8:40am **2D+EM+MI+MN-MoM-2 Topological Toughening of Graphene and other 2D Materials***, **Bo Ni**,* Brown university*; H Gao,* Brown University

It has been claimed that graphene, with the elastic modulus of 1 TPa and theoretical strength as high as 130 GPa, is the strongest material. However, from an engineering point of view, it is the fracture toughness that determines the actual strength of materials, as crack-like flaws (i.e., cracks, holes, notches, corners, etc.) are inevitable in design, fabrication and operation of practical devices and systems. Recently, it has been demonstrated that graphene has very low fracture toughness, in fact close to that of ideally brittle solids. These findings have raised sharp questions and are calling for efforts to explore effective methods to toughen graphene. Recently, we have been exploring the potential use of topological effects to enhance the fracture toughness of graphene. For example, it has been shown that a sinusoidal graphene containing periodically distributed disclination quadrupoles can achieve a mode I fracture toughness nearly twice that of pristine graphene. Here we report working progresses on further studies of topological toughening of graphene and other 2D materials. A phase field crystal method is adopted to generate the atomic coordinates of material with specific topological patterns. We then perform molecular dynamics simulation of fracture in the designed samples, and observe a variety of toughening mechanisms, including crack tip blunting, crack trapping, ligament bridging, crack deflection and daughter crack initiation and coalescence.

9:00am **2D+EM+MI+MN-MoM-3 Ferroelectric Domain Control of Photoluminescence in Monolayer WSe$_2$ / PZT Hybrid Structures***, **Berry Jonker**, C Li, K McCreary,* Naval Research Laboratory

Single monolayer transition metal dichalcogenides (TMDs) exhibit exceptionally strong photoluminescence dominated by a combination of distinct neutral and charged exciton contributions. The dielectric screening is very low due to their two-dimensional character relative to bulk material, and their properties are thus strongly affected by their immediate environment. Because the exciton and trion binding energies are very large (~ 600 meV and ~30 meV, respectively), these characteristic emission features persist to room temperature. The samples were fabricated by mechanically transferring large area monolayer WS$_2$ grown by a CVD process onto 100 nm thick lead zirconium titanate (PZT) films on a conducting *n*-type strontium titanate wafer. We show here that the surface charge associated with ferroelectric domains patterned into the PZT film with a conductive atomic force microscope laterally control the spatial distribution of neutral and charged exciton populations in the adjacent WS$_2$ monolayer [1]. This is manifested in the intensity and spectral composition of the photoluminescence measured in air at room temperature from the areas of WS$_2$ over a ferroelectric domain with polarization dipole pointed either out of the surface plane or into the surface plane. The photoluminescence from areas of the WS$_2$ over up polarization domains in the PZT are dominated by neutral exciton emission, while those over down domains are dominated by trion emission, consistent with the corresponding charge produced by the domains at the WS$_2$ / PZT interface. The hysteretic character of ferroelectric materials means that the TMD properties can be selectively reconfigured in a nonvolatile manner by changing the state of the ferroic substrate. This approach enables spatial modulation of TMD properties with a spatial resolution determined by the polarization domains in the underlying ferroelectric layer, with the potential for fabrication of lateral quantum dot arrays or *p-n* junctions in any geometry of choice.

[1] C.H. Li, K.M. McCreary and B.T. Jonker, *ACS Omega* 1, 1075 (2016).

This work was supported by core programs at NRL and the NRL Nanoscience Institute, and by the Air Force Office of Scientific Research #AOARD 14IOA018-134141.

9:20am **2D+EM+MI+MN-MoM-4 Mechanical Instability-driven Architecturing of Atomically-thin Materials***, **SungWoo Nam**,* University of Illinois at Urbana-Champaign

Mechanical deformations, such as buckling, crumpling, wrinkling, collapsing, and delamination, are usually considered threats to mechanical integrity which are to be avoided or reduced in the design of materials and structures. However, if materials systems and applied stresses are carefully controlled, such mechanical instabilities can be tailored to deterministically create functional morphologies that can enable powerful new functions. In particular, in atomically-thin material systems with ultralow bending stiffness, such as graphene, mechanical deformations enable new structural properties and device-level functionalities which surpass the limits of bulk material systems. In this talk, I will present our manufacturing technique on controlled deformation and straining of atomically-thin materials, and the emergent materials properties and applications of such deformed and strained atomically-thin materials. First, I will introduce shrink-manufacturing approaches to enable controlled deformation of atomically-thin materials. Second, I will introduce a wide range of new material properties enabled by the new class of 'architectured atomically-thin materials'. I will discuss the surface plasmonics enabled by crumpled topographies of graphene and will further discuss shape reconfigurability which opens the door to tunable plasmonic resonance of crumpled graphene. In addition, I will share our ongoing research efforts on strained superlattice for the modulation of electronic properties. Third and last, I will present our work on adaptive/conformal and multifunctional electronics based on mechanically deformed atomically-thin materials. Our optoelectronic sensor is based exclusively on graphene and transforms the two dimensional material into three dimensional (3D) crumpled structures. This added dimensionality enhances the photoabsorption of graphene by increasing its areal density with a buckled 3D structure, which simultaneously improves device stretchability and furthermore enables strain-tunable photoresponsivity. Our approach to manufacturing architectured atomically-thin materials offers a unique avenue for enabling new materials properties and engineering of advanced device functions.

9:40am **2D+EM+MI+MN-MoM-5 Excitons and Exciton Complexes in Transition Metal Dichalcogenide Monolayers***, **Mark Hybertsen**,* Brookhaven National Laboratory **INVITED**

Ultra-thin semiconductor crystals, realized from transition metal dichalcogenides and other Van der Waals materials, exhibit fascinating optical properties. In the limit of a single monolayer of material, the Coulomb interactions between the optically excited electrons and holes are particularly strong and specifically deviate in functional form from that familiar from bulk semiconductors (1/εr) [1]. In combination with the reduced dimensionality, the resultant interaction effects are an order of magnitude stronger than those that were previously observed in quantum well structures realized in epitaxially grown multilayers. The lowest energy excitations created by optical excitation are bound electron-hole pairs (excitons). The binding energy is on the 0.5 eV scale and the ladder of bound state energies observed deviate significantly from the spectrum predicted by the conventional hydrogenic model [2]. In the presence of excess carriers, the excitons also form a bound complex with either an excess electron or hole (trions) [1]. As the density of optically excited excitons is increased, pairs of bound excitons form (biexcitons), with a clear spectroscopic signature [3]. All of these characteristics of excitons and exciton complexes in transition metal dichalcogenides can be understood directly from the strong and modified form of the Coulomb interaction, including both the role of the environment and the impact of the intrinsic screening response of the material. In particular, a model Hamiltonian can be fully determined from microscopic inputs and solved for the properties of the observed excitons and associated complexes. Variational solutions are semiquantitative while supplying insight. A Monte Carlo approach solves the model Hamiltonian numerically exactly and gives quantitative relationships among the exciton and exciton complex binding energies [4]. Extensions of these approaches to understand excited states in more complex combinations of such layered materials will also be discussed.

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[1] T. C. Berkelbach, M. S. Hybertsen, and D. R. Reichman, Phys. Rev. B **88**, 045318 (2013).

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[3] Y. You, X.-X. Zhang, T. C. Berkelbach, M. S. Hybertsen, D. R. Reichman, and T. F. Heinz, Nat. Phys. **11**, 477 (2015).

[4] M. Z. Mayers, T. C. Berkelbach, M. S. Hybertsen, and D. R. Reichman, Phys. Rev. B **92**, 161404 (2015).

11:00am **2D+EM+MI+MN-MoM-9 Mechanical Properties of Polycrystalline and Defective Graphene***, **Joseph Gonzales**, I Oleynik, J Willman,* University of South Florida*; R Perriot,* Los Alamos National Laboratory

Experimental investigation of mechanical properties indicates that the polycrystalline graphene grown by chemical vapor deposition is as strong as pristine. Recent experiments involving nanoindentation of graphene have also demonstrated counterintuitive increasing of Young's modulus with increasing concentrations of point defects. Using accurate description of interatomic interactions provided by novel screened environment-dependent bond order, (SED-REBO) potential, we performed large-scale molecular dynamics investigations of mechanical properties of polycrystalline and defective graphene samples under conditions mimicking nano-indentation AFM experiments. The atomically resolved characterization of the stress and strain distributions under indenter are used to understand fundamental mechanisms of graphene strength and failure. The breaking strength, the crack initiation and propagation are investigated as a function of the grain boundary structure, grain size distribution, concentration of point defects as well as the position of the indenter in respect to these extended and point defects.

11:20am **2D+EM+MI+MN-MoM-10 Properties of Single Layer Transition Metal Dichalcogenides Grown by Van der Waals Epitaxy***, **Matthias Batzill**,* University of South Florida **INVITED**

It is well documented that the electronic properties of transition metal dichalcogenides (TMDs) vary as their dimensions are reduced to a single layer. Also, variations depending on the substrate have been reported. In our studies we grow single- to few- layers of TMDs by molecular beam epitaxy on van der Waals substrates (mainly HOPG or bulk-$MoS_2$). Despite the weak interactions between the monolayer and the substrate the film grows rotational aligned so that a film exhibits a single crystal orientation. This enables for example electronic structure characterization by angle resolved photoemission spectroscopy. The versatile growth procedure allows us to characterize many materials systems. First we discuss the role of the substrate for semiconducting TMDs. We study the electronics structure variation for $MoSe_2$ grown on another TMD ($MoS_2$) and compare it with that grown on HOPG. While the band dispersion of $MoSe_2$ on HOPG resembles the expectations for free-standing $MoSe_2$ it is modified for $MoSe_2/MoS_2$ due to interlayer hybridization of the chalcogen p-orbitals. A big advantage of MBE growth in vacuum is that it enables the synthesis and study of more reactive systems – like most metallic TMDs. Thus, in the second part of this talk we investigate the properties of single layer $TiSe_2$. $TiSe_2$ is an unconventional charge density wave (CDW) material whose charge density wave transition has been associated with an excitonic insulator phase. Such an excitonic insulator is formed spontaneously if the excitonic binding energy exceeds the band gap and thus formation of excitons may become the ground state. By scanning tunneling spectroscopy we observe significant increase in the CDW-band gap opening at the Γ-point for the monolayer compared to few-layer materials. Furthermore, the opening of the gap varies with the substrate material, consistent with expectations for excitonic binding energies. Interestingly, we observe coherence peaks in the tunneling spectra below 50 K suggesting the formation of an excitonic condensate.

## Spectroscopic Ellipsometry Focus Topic
## Room 9 - Session EL+AS+EM+TF-MoM

### Application of SE for the Characterization of Thin Films and Nanostructures

**Moderator:** Tino Hofmann, University of North Carolina at Charlotte

8:20am **EL+AS+EM+TF-MoM-1 Ultra-thin Plasmonic Metal Nitrides: Optical Properties and Applications***, **Alexandra Boltasseva**,* Purdue University **INVITED**

Transition metal nitrides (e.g. TiN, ZrN) have emerged as promising plasmonic materials due to their refractory properties and good metallic properties in the visible and near infrared regions. Due to their high melting point, they may be suitable for high temperature nanophotonic applications. We have performed comprehensive studies of the temperature induced deviations to the dielectric function in TiN thin films. The studies were conducted on 30 nm, 50 nm, and 200 nm TiN films on sapphire substrates at temperatures up to 900 0C in the wavelength range 350-2000 nm using a custom built in-situ high temperature ellipsometry setup. The results were fitted with a Drude-Lorentz model consisting of one Drude oscillator and 2 Lorentz oscillators. As the temperature is elevated, the real and imaginary parts both begin to degrade. However, the deviations to the optical properties of TiN are significantly smaller compared to its noble metal counterparts, with no structural degradation in the TiN films. In addition to high temperature applications, TiN could also be a potential material platform for investigating light-matter interactions at the nanoscale, since high quality, continuous films of TiN can be grown on substrates such as MgO and c-sapphire down to just a few monolayers. Ultrathin TiN films with thicknesses of 2, 4, 6, 8, and 10 nm were grown on MgOusing DC reactive magnetron sputtering, resulting in high quality films with low roughness. The changes in the linear optical properties were investigated using variable angle spectroscopic ellipsometry at angles of 50° and 70° for wavelengths from 400 nm to 2000 nm. A Drude-Lorentz model consisting of one Drude oscillator and one Lorentz oscillator was used to fit the measurements. As the thickness decreased, an increase in the losses and a decrease in the plasma frequency was observed. However, the films remained highly metallic even at 2nm, demonstrating that they could be used for nanophotonicapplications, including nonlinear optical devices and actively tunable plasmonic devices.

9:00am **EL+AS+EM+TF-MoM-3 Magnetron Sputtering of TiN Coatings: Optical Monitoring of the Growth Process by Means of Spectroscopic Ellipsometry***, **Jiri Bulir**, J More Chevalier, L Fekete, J Remiasova, M Vondracek, M Novotny, J Lancok,* Institute of Physics ASCR, Czech Republic

The plasmonic applications requires search for novel materials with metal-like optical properties and low optical losses. Transition metal nitrides such as TiN, TaN, ZrN, HfN, NbN exhibit metallic properties depending on concentration of free-carrier of charge. Their plasmonic properties can be tuned by deposition parameters controlling the film structure and the stechiometry.

In this work, we deal with study of growth process of TiN films. The films are grown by RF magnetron sputtering on fused silica, silicon and MgO substrates at substrate temperature ranging from 20°C to 600°C. The growth process is monitored using in-situ spectral ellipsometer in spectral range from 245 to 1690 nm. The ellipsometric data, which are obtained during the deposition process, are attentively analysed using mathematical models based on Drude-Lorentz oscillators.

The Lorentz oscillators are used for description of interband transition in ultraviolet and visible spectral range, whereas the Drude oscillator describes the free-electron behavior in the infrared spectral range. We show that the free-electron behavior is affected by thickness of the ultrathin coatings due to electron scattering effects at the interfaces. Number of physical parameters such as free-electron concentration, Drude relaxation time and electrical conductivity is estimated at each stage of the deposition process by analysis of dielectric functions using the mentioned model. The resulting evolution of the electrotransport properties during the TiN film growth is presented. Special attention is devoted to the initial nucleation stage when the free-electron behaviour is significantly influenced by the interface between the substrate and the TiN film. Based on evolution of electrotransport properties, we discuss differences between polycrystalline growth of TiN film on Si and fused silica substrates and epitaxial growth on MgO substrates.

The accomplished TiN coatings are analyzed using infrared ellipsometer operating in spectral range from 1.7µm to 30µm where the optical constants are infuenced most importantly by free-electron behaviour. The obtained results are compared with those obtained by the in-situ ellipsometer. Special attention is focused on scattering of free electrons at grain boundaries and at the TiN layer interfaces. The estimated parameters are correlated with structure changes such as grain coarsening and surface morphology. The crystallinity is analysed by X-ray Difractometry. The surface morphology of the completed coatings is studied using Atomic Force Microscopy and Scanning Electron Microscopy. The TiN film stechiometry is estimated by X-ray Photoemission Spectroscopy.

9:20am **EL+AS+EM+TF-MoM-4 Variable Temperatures Spectroscopic Ellipsometry Study of the Optical Properties of InAlN/GaN Grown on Sapphire***, Y Liang,* Guangxi University, China*; H Gu,* Huazhong University of Science and Technology, China*; J Xue,* Xidian University, China*; **Chuanwei Zhang**,* Huazhong University of Science and Technology, China*; Q Li,* Guangxi University, China*; Y Hao,* Xidian University, China*; S Liu,* Huazhong University of Science and Technology, China*; Q Yang, L Wan, Z Feng,* Guangxi University, China

Indium aluminum nitride (InAlN), a prospective material for lattice matched confinement layer, possesses the potential to improve the reliability and performance of high electron mobility transistors (HEMTs).[1] One of the important advantages of InAlN alloy is the possibility of growing in-plane lattice-matched to GaN for an indium content of around 17%. However, the bandgap we expected is hindered by the growth of high-quality InAlN films due to the phase separation and nonuniform composition distribution.[1-2]

In this work, InAlN/GaN heterostructures, grown by pulsed metal organic chemical vapor deposition (PMOCVD) on c-plane sapphire substrates, were investigated by a dual rotating-compensator Mueller matrix ellipsometer (ME-L ellipsometer, Wuhan Eoptics Technology Co. Ltd., China). The experimental data (Ψ and Δ), covering the wavelength (λ) range from 193 nm up to 1700 nm at 1 nm step or energy (E) from 0.73 eV to 6.43 eV, were obtained by variable temperatures spectroscopic ellipsometric (VTSE) in three angles (50°, 55° and 60°). The Eoptics software was utilized to fit VTSE data using Tauc-Lorentz multiple oscillator modes. By analyzing the fitting results, the optical constants of the InAlN at variable temperatures (25℃-600℃) were obtained. The peak value of the refractive index increases from 269 nm to 284 nm with increasing temperature. The bandgaps are 4.57 eV and 4.35 eV at the temperature 25℃and 600℃, respectively. These results demonstrated that InAlN/GaN has a high thermal stability, scilicet no significant performance degradation in high temperature environment.

Reference

[1] Wenyuan Jiao, Wei Kong, Jincheng Li et al, Characterization of MBE-grown InAlN/GaN heterostructures valence band offsets with varying In composition, AIP ADVANCES 6, 035211 (2016).

[2] JunShuai Xue, JinCheng Zhang, Yue Hao, Investigation of TMIn pulse duration effect on the properties of InAlN/GaN heterostructures grown on sapphire by pulsed metal organic chemical vapor deposition, Journal of Crystal Growth 401, 661 (2014).

9:40am **EL+AS+EM+TF-MoM-5 Optical Properties of $Cs_2AgIn_{(1-x)}Bi_xCl_6$ Double Perovskite Studied by Spectroscopic Ellipsometry***, **Honggang Gu**, S Li, B Song, J Tang, S Liu,* Huazhong University of Science and Technology, China

During the past several years, the organic-inorganic lead halide perovskites ($APbX_3$, A = $CH_3NH_3$ or $NH_2CHNH_2$, X = Cl, Br, or I) have been promising materials for photovoltaic, photoelectric -detecting and light-emitting devices due to their outstanding photoelectric properties, such as broad absorption range, high quantum efficiency, ultrafast charge generation, high charge carrier mobility and long charge carrier lifetime and diffusion length. However, there are two remaining challenges that need to be addressed in order to apply these materials to photoelectric productions, namely the compound stability and the presence of lead. Most recently, lead-free metal halide double perovskites, such as $Cs_2AgBiCl_6$ and $Cs_2AgInCl_6$, have attracted extensive attention because of their nontoxicity and relative air-stability. In the study and application of these perovskite materials, the knowledge of their optical properties, such as the bandgap and the basic optical constants, is of great importance to predict the photoelectric characteristics and dig the potential of the materials.

Spectroscopic ellipsometry (SE) has been developed as a powerful tool to characterize the optical properties as well as structure parameters of novel materials, thin films and nanostructures. In this work, we study the optical properties of $Cs_2AgIn_{(1-x)}Bi_xCl_6$ perovskites by a spectroscopic ellipsometer (ME-L ellipsometer, Wuhan Eoptics Technology Co., Wuhan, China). The refractive index and the extinction coefficient of $Cs_2AgIn_{(1-x)}Bi_xCl_6$ with different composition coefficient $x$ of bismuth are determined by the ellipsometer over the wavelength range of 250-1000nm. We find that the presence of bismuth introduces two critical points in the optical constant spectra of the perovskites, i.e., 315nm and 382nm in the refractive index spectra and 300nm and 375nm in the extinction coefficient spectra, respectively. Moreover, there is a red shift in the bandgaps and significant increase in both the refractive index and the extinction coefficient with the increase of composition coefficient $x$ of bismuth.

10:00am **EL+AS+EM+TF-MoM-6 Charge Carrier Dynamics of Aluminum-doped Zinc Oxide Deposited by Spatial Atomic Layer Deposition***, **Daniel Fullager**, G Boreman, T Hofmann,* University of North Carolina at Charlotte*; C Ellinger,* Eastman Kodak Company

Transparent conductors for displays, backplanes, touchscreens and other electronic devices are an area of active research and development; in this manner, aluminum-doped zinc oxide (AZO) has shown promise as an ITO replacement for some applications. Although there have been numerous reports on the optical properties and electrical conductivity of AZO, there has not yet been a Kramers-Kronig consistent dispersion model fully describing the charge carrier dynamics. In this presentation, we will report on the model dielectric function of AZO from the combination of UV-Vis and IR spectroscopic ellipsometry. A model dielectric function that describes the optical response over this wide spectral range will be presented and discussed. In particular, we will present a comparison between the commonly used extended Drude models and the dielectric function developed here in light of results obtained from density functional theory calculations.

The AZO films analyzed in this study were deposited using a spatial atomic layer deposition (SALD) process. While AZO can be deposited by several techniques, including sputtering, chemical vapor deposition (CVD), and atomic layer deposition (ALD), ALD does allow for the greatest ability to control the aluminum-doping level of AZO. However, the range of substrate sizes and form factors addressable by traditional chamber ALD are limited. Conversely, spatial ALD (SALD) is an atmospheric pressure, roll-compatible ALD process that enables the materials property control of ALD to be translated into a wider range of applications spaces. Furthermore, the use of selective area deposition in a “patterned-by-printing” approach enables the high-quality AZO deposited by SALD to be easily patterned, offering an integrated and facile path for manufacturing optical and electronic devices.

10:40am **EL+AS+EM+TF-MoM-8 Broad Range Ellipsometry Shining Light onto Multiphase Plasmonic Nanoparticles Synthesis, Properties and Functionality***, **Maria Losurdo**,* CNR-NANOTEC, Italy **INVITED**

How rich are the physics, interface chemistry and optical properties associated with the surface plasmons of metal nanostructures and their potential for manipulating light at the nanoscale! For many technological applications nanoparticles (NPs) are supported on a substrate, and at the nanoscale, interaction and interfaces with the support become very important. We have demonstrated that the substrate/NPs interaction is the key to engineering not only the shape but also the crystalline phase of NPs.

This contribution will present and explore fundamental and applied aspects of multiphase core-shell plasmonic NPs supported on substrates of technological interest using various diagnostic tools, which comprise: (i) spectroscopic ellipsometry spanning the THz, IR, visible, and UV wavelength ranges, (ii) variable angle Muller Matrix ellipsometry to qualify size effects on anisotropy and depolarization of samples, (iii) *in-situreal-time* spectroscopic ellipsometry to understand growth and tailor particle size which ultimately controls the plasmon resonance, and (iv) various imaging and microscopies techniques to elucidate the interplay between the nanostructure of multiphase nanoparticle and their functionality.

The case studies involve liquid-shell/solid-core plasmonic NPs (Ga, Ga/Mg), plasmon-catalytic core/shell Ga/Pd and plasmon-magnetic Ni/Ga NPs supported on various substrates (glass, plastics, sapphire) that control their crystalline phases.

We will start with a description of the *real-time* ellipsometry capabilities in monitoring the growth of those multiphase core/shell NPs to detect the formation of the various phases in situ and to control the resulting plasmon resonance.

The discussion then will shifts to a description of fundamental of thermodynamics of substrate supported multiphase NPs and how their growth dynamics is controlled by the interface energies, and how those new phenomena can be highlighted by real-time ellipsometry.

Ex-situ corroborating measurements of Mueller-matrix ellipsometry and hyperspectral cathodoluminescence spectroscopy and imaging will be presented to discuss phenomena of depolarization and of interaction of NPs resulting from the self-assembly.

Finally, since those NPs enable active plasmonics, we demonstrate the implications of the multi-phase nature of NPs, as well as solid-liquid phase coexistence on the plasmon resonance (LSPR) of supported NPs and on its exploitation to follow in real time phenomena in their application in catalysis (hydrogen storage and sensing) and optomagnetism and possible future directions.

*The contribution of the H2020 European programme under the project TWINFUSYON (GA692034) is acknowledged*

11:20am **EL+AS+EM+TF-MoM-10 Use of Evolutionary Algorithms for Ellipsometry Model Development and Validation using Eureqa***, **Neil Murphy**,* Air Force Research Laboratory*; L Sun,* General Dynamics Information Technology*; J Jones,* Air Force Research Laboratory*; J Grant,* Azimuth Corporation

Eureqa, developed by Nutonian Inc., is a proprietary modeling engine based on automated evolutionary algorithms. In this study, we utilized Eureqa to parameterize both the amplitude and phase difference data for reactively sputtered thin films. Specifically, evolutionary algorithms are used to develop and validate models for fitting raw ellipsometric data for a variety of optical materials including $SiO_2$, Ta-$_2O_5$, and Aluminum Zinc Oxide. These films, deposited using pulsed DC magnetron sputtering, were deposited on both silicon and fused quartz substrates, and measured using a J.A. Woollam VASE system. The resulting models are then compared to traditional models that are currently utilized to fit the candidate materials systems.

11:40am **EL+AS+EM+TF-MoM-11 Excitonic Effects on the Optical Properties of Thin ZnO Films on Different Substrates***, **Nuwanjula Samarasingha**, Z Yoder, S Zollner,* New Mexico State University*; D Pal, A Mathur, A Singh, R Singh, S Chattopadhyay,* Indian Institute of Technology Indore, India

The presence of excitonic features in the optical constants of bulk semiconductors and insulators has been known for many years. In Si, Ge, and GaAs, the $E_1$ critical points are strongly enhanced by two-dimensional excitons. Three-dimensional excitons have been seen in ellipsometry spectra for GaP and Ge. In addition to these semiconductors, wide band gap materials like ZnO exhibit strong excitonic features in the dielectric function ($\varepsilon$) which is directly related to the electronic band structure. The top valence band at the $\Gamma$ point in the Brillouin zone is split into three bands by spin orbit and crystal field splitting. The corresponding free exciton transitions between the lowest conduction band and these three valence bands are denoted by A, C ($\Gamma_7$ symmetry) and B ($\Gamma_9$ symmetry). The transition from the B subband is forbidden for light polarized parallel to the optical axis (extraordinary dielectric function). ZnO is attractive for optoelectronic device applications due to its large excitonic binding energy of 60 meV at room temperature.The influence of this excitonic absorption on $\varepsilon$ was described by Tanguy [1].

Here we investigate the behavior of excitons in c-oriented ZnO thin films grown on Si (smaller band gap than ZnO) and $SiO_2$ (larger band gap than ZnO) substrates using variable angle spectroscopic ellipsometry and FTIR ellipsometry. We also performed X-ray diffraction (XRD), X-ray reflectivity (XRR), and atomic force microscopy (AFM) to characterize the structural properties of our ZnO films.

In a thin epitaxial layer on a substrate with a different band gap, the wave functions of the electron and hole are strongly modified. In ZnO (band gap 3.37 eV) grown on a large-gap $SiO_2$ substrate (type-I quantum well), both the electron and the hole are confined, which leads to an increase in the dipole overlap matrix element. Therefore, the real and imaginary part of $\varepsilon$ of thin ZnO layers on $SiO_2$ are much larger than in the bulk and increase monotonically with decreasing thickness.

On the other hand, in a staggered type-II quantum well (ZnO on Si), either the electron is confined, or the hole, but not both. Therefore, the overlap dipole matrix element is strongly reduced. Therefore, $\varepsilon$ of thin ZnO layers on Si is much smaller than in the bulk and decreases monotonically with decreasing thickness. We will fit our ellipsometric spectra by describing the dielectric function of ZnO using the Tanguy model [1]. We will analyze the dependence of the excitonic Tanguy parameters on quantum well thickness and substrate material.

Reference:

[1] C. Tanguy, Phys. Rev. Lett. **75**, 4090 (1995).

## Electronic Materials and Photonics Division
## Room 14 - Session EM+MI+TF-MoM

## Growth, Electronic, and Magnetic Properties of Heusler Compounds

**Moderators:** Rehan Kapadia, University of Southern California, Seth King, University of Wisconsin - La Crosse

8:20am **EM+MI+TF-MoM-1 Semiconducting Half-Heusler Heterostructures Grown by Molecular Beam Epitaxy***, **Anthony Rice**, S Harrington, D Pennachio, M Pendharkar, C Palmstrøm,* University of California at Santa Barbara

Half-Heusler (hH) compounds are an attractive family of materials for a number of applications due to their wide range of properties, including half-metallic ferromagnetism and topologically non-trivial surface states. Additionally, those containing 18 valence electrons per formula unit are predicted to show a semiconducting band gap [1]. This suggests the possibility of a single multifunctional material composed of compounds with the same crystal structure throughout which makes use of the diverse hH properties not accessible by traditional III-V technology as well as more traditional band gap engineering.

In this presentation, the heterointerface formed between the 18 valence electron semiconducting hHs, CoTiSb and NiTiSn, is investigated. Layered structures with both NiTiSn and CoTiSb, have been successfully grown on MgO(001) substrates using molecular beam epitaxy. Transmission electron microscopy and X-ray diffraction (XRD) data suggest separate layers with sharp interfaces. X-ray photoelectron spectroscopy (XPS) data shows no evidence of intermixing, with component peaks attenuating as expected. XPS is used to measure the valence band offset, which suggests a type-I heterojunction.

Through the use of CoTiSb buffer layers, the integration of NiTSn with III-V substrates is demonstrated. Previous attempts at direct growth of NiTiSn on III-Vs has proven unsuccessful due to the high reactivity of nickel with III–Vs. Reflection high-energy electron diffraction intensity oscillations during growth are observed for these structures, consistent with layer-by-layer growth. XRD interference fringes suggest abrupt interfaces. Higher quality NiTiSn is ultimately achieved, with lower carrier concentrations and higher mobility. Interface transport, both laterally and vertically, is also explored.

This work was supported in part by the Vannevar Bush Faculty Fellowship (ONR-N0014-15-1-2845) and NSF-MRSEC (DMR-1121053). The UCSB MRL Shared Experimental Facilities are supported by the MRSEC Program of the NSF under Award No. DMR 1121053; a member of the NSF-funded Materials Research Facilities Network. A part of this work was performed in the UCSB Nanofabrication Facility which is a part of the NSF funded National Nanotechnology Infrastructure Network.

[1] T. Graf, C. Felsar, and S. Parkin. Progress in Solid State Chemistry 39 (2011) 1-50

8:40am **EM+MI+TF-MoM-2 Towards Topotronics: Combining Chemical Potential Tuning and Strain Engineering to Realize Surface Dominated Transport in Topological Heusler Thin Films***, **Shouvik Chatterjee**, J Logan, N Wilson, M Pendharkar, C Palmstrøm,* University of California at Santa Barbara

Heusler compounds have emerged as an exciting material system where realization of functional and tunable novel topological phases might be possible[1-4]. PtLuSb is one such compound that has been shown to host topologically non-trivial surface states[5]. However, being a semi-metal without a bulk band gap, exotic transport and thermodynamic properties expected from topological surface states are obscured by contributions from trivial bulk carriers that limits possible device applications[6]. Furthermore, natural defects in the compound leads to unintentional p-type doping resulting in the surface Dirac point lying above the chemical potential[5,6,7].

In this talk, I will present our efforts to address both these issues by a combination of carrier doping and substrate induced bi-axial strain to shift the chemical potential and attempt to open up a bulk gap, respectively. I will show experimental evidence of chemical potential tuning in Au alloyed $Pt_{1-x}Au_xLuSb$ thin films where the surface Dirac point can be pushed below the Fermi level. In addition, it is possible to open a bulk-band gap by application of compressive bi-axial strain on thin films synthesized on lattice mismatched substrates. Realization of surface dominated transport in topological Heusler thin films will open up avenues for realization of many exotic phenomena such as quantum anomalous Hall effect[8], axion insulators[9], topological superconductivity[10] and their potential device applications.

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9:00am **EM+MI+TF-MoM-3 Topology, Magnetism, and Superconductivity in Ternary Half-Heusler Semimetals***, **Johnpierre Paglione**,* University of Maryland, College Park **INVITED**

In materials with non-centrosymmetric crystallographic structures, it has long been known that the lack of inversion symmetry can give rise to odd-parity spin-triplet pairing states. We report superconductivity and magnetism in a new family of topological semimetals, the ternary half Heusler compounds RPtBi and RPdBi (R : rare earth). In this series, tuning of the rare earth f-electron component allows for simultaneous control of both lattice density via lanthanide contraction, as well as the strength of magnetic interaction via de Gennes scaling, allowing for a unique tuning of both the normal state band inversion strength, superconducting pairing and magnetically ordered ground states. Antiferromagnetism with ordering vector (0.5,0.5,0.5) occurs below a Néel temperature that scales with de Gennes factor, while a superconducting transition is simultaneously linearly suppressed. With superconductivity appearing in a system with non-centrosymmetric crystallographic symmetry as well as p-orbital derived spin-3/2 quasiparticles, the possibility of high-spin Cooper pairing (i.e. beyond triplet) with non-trivial topology analogous to that predicted for the normal state electronic structure provides a unique and rich opportunity to realize both predicted and new exotic excitations in topological materials.

9:40am **EM+MI+TF-MoM-5 Electron Counting, Surface Reconstructions, and Electronic Structure of 18 Electron Half Heuslers***, **Jason Kawasaki**,* University of Wisconsin - Madison*; A Janotti,* University of Delaware*; C Palmstrøm,* University of California at Santa Barbara

Half Heusler compounds (composition *ABC*) show great promise for the development of earth abundant thermoelectrics, half metallic ferromagnets for spin injection, and topological heterostructures. In these applications, the electronic structure of surfaces and interfaces are critical to materials performance. However, little is known about how and why the surfaces of these materials reconstruct or their direct effect on electronic properties. Using a combination of molecular beam epitaxy, angle resolved and core level photoemission, scanning tunneling microscopy, and density functional theory (DFT), we investigate the stability, reconstructions, and electronic surface states on the (001) surfaces of CoTiSb, NiTiSn, and FeVSb. These compounds are representative of a large class of 18 valence electron Half Heuslers that are expected to be semiconducting. We find that reconstructions in these compounds are characterized by *C* site (group IV or V) dimerization, as in III-V semiconductors, and this dimerization coincides with *B* site vacancies at the surface. We explain these trends using a simple electron counting model, and predictions from the model are in good agreement with both the experimental data and with DFT calculations. Our combined theoretical and experimental studies provide a rationale for understanding and controlling reconstructions and resultant electronic surface states in Heuslers.

10:00am **EM+MI+TF-MoM-6 Computational Investigation of Heusler Compoundss for Spintronic Applications***, **Jianhua Ma**,* University of Virginia*; W Butler,* University of Alabama

We present first-principles density functional calculations of the electronic structure, magnetism, and structural stability of 378 *XYZ* half-Heusler, 405 $X_2YZ$ inverse-Heusler, 576 $X_2YZ$ full-Heusler compounds. We find that a “Slater-Pauling gap” in the density of states in at least one spin channel is a common feature in Heusler compounds. We find that the presence of such a gap at the Fermi energy in one or both spin channels contributes significantly to the stability of a Heusler compound. We calculate the formation energy of each compound and systematically investigate its stability against all other phases in the open quantum materials database (OQMD). We represent the thermodynamic phase stability of each compound as its distance from the convex hull of stable phases in the respective chemical space and show that the hull distance of a compound is a good measure of the likelihood of its experimental synthesis. We find low formation energies and mostly correspondingly low hull distances for compounds with X = Co, Rh, or Ni, Y = Ti or V, and Z = P, As, Sb, or Si in half-Heulser compounds. In the half-Heusler family, we identify 26 18-electron semiconductors, 45 half-metals, and 34 near half-metals with negative formation energy that follow the Slater-Pauling rule of three electrons per atom. In the inverse-Heusler family, we identify 14 asymmetric 18-electron semiconductors, 50 half-metals, and 42 near half-metals with negative formation energy. In the full-Heusler family, we identify 8 24-electron semiconductors and 23 half-metals with negative formation energy. Our calculations predict several new, as-yet unknown, thermodynamically stable phases, which merit further experimental exploration—RuVAs, CoVGe, FeVAs in the half-Heusler structure, and NiScAs, RuVP, RhTiP in the orthorhombic MgSrSi-type structure. Further, two interesting zero-moment half-metals, CrMnAs and MnCrAs, are calculated to have negative formation energy. In addition, our calculations predict a number of hitherto unreported semiconducting (e.g., CoVSn and RhVGe), half-metallic (e.g., RhVSb), and near half-metallic (e.g., CoFeSb and CoVP) half-Heusler compounds to lie close to the respective convex hull of stable phases, and thus may be experimentally realized under suitable synthesis conditions, resulting in potential candidates for various semiconducting and spintronics applications.

11:00am **EM+MI+TF-MoM-9 Growth, Electronic, and Magnetic Properties of Half-Heusler $CoTi_{1-x}Fe_xSb$***, **Sean Harrington**, A Rice, T Brown-Heft, A McFadden, M Pendharkar,* University of California at Santa Barbara*; O Mercan, L Çolakerol Arslan,* Gebze Technical University, Turkey*; C Palmstrøm,* University of California at Santa Barbara

Recent predictions suggest the semiconducting half-Heusler compound, CoTiSb, exhibits half-metallicity when substitutionally alloyed with Fe. However, to date, few studies have examined the growth of high-quality single crystal thin films of Fe-alloyed CoTiSb. Here, we report the epitaxial growth of the substitutionally alloyed half-Heusler series $CoTi_{1-x}Fe_xSb$ by molecular beam epitaxy and the influence of Fe on the structural, electronic, and magnetic properties. $CoTi\text{-}_{1-x}Fe_{x}\text{-}Sb$ epitaxial films are grown on InAlAs grown on InP (001) substrates for concentrations $0 \leq x \leq 1$. The films are epitaxial and single crystalline, as measured by reflection high-energy electron diffraction and X–ray diffraction. For films with higher Fe content, a lower growth temperature is necessary to minimize interfacial reactions. Using *in-situ* X-ray photoemission spectroscopy, only small changes in the valence band spectra from pure CoTiSb are detected. For films with $x \geq 0.05$, ferromagnetism is observed in SQUID magnetometry with a Curie temperature >400K. The saturation magnetization of the series increases linearly with Fe content as 3.4 $\mu_B$/Fe atom. In comparison, there is a much smaller magnetic moment when the Fe is substituted on the Co site ($Co_{1-x}Fe_{x}$-Ti-Sb) indicating a strong dependence of the magnetic moment with site occupancy. A cross over from both in-plane and out-of-plane magnetic moments to only in-plane occurs for higher concentrations of Fe. Ferromagnetic resonance indicates a transition from weak to strong interaction as Fe content is increased. Temperature dependent transport shows a gradual semiconductor to metal transition with thermally activated behavior for $x \leq 0.3$. Anomalous Hall effect and magneto resistance are investigated for the x=0.3 and x=0.5 films revealing large differences in the electronic scattering mechanisms and transport behavior depending on Fe content.

11:20am **EM+MI+TF-MoM-10 High Spin-Polarization and Perpendicular Magnetic Anisotropy in Single-Crystal Full-Heusler $Co_2MnAl/Fe_2MnAl$ Superlattice***, **Tobias Brown-Heft**, A McFadden, J Logan,* University of California at Santa Barbara*; C Guillemard,* University of Lorraine, France*; P Le Fevre, F Bertran,* Synchrotron SOLEIL, France*; S Andrieu,* University of Lorraine, France*; C Palmstrøm,* University of California at Santa Barbara

Ferromagnetic contacts are used as a source of spin-polarized current in many spintronic devices. Desired properties for ferromagnetic contacts used in magnetic tunnel junctions and other next-generation memory elements are perpendicular magnetic anisotropy and 100% spin polarization at the Fermi level (half-metallicity). Heusler compounds are strong candidates for this purpose as many have been predicted and observed to be half-metals (e.g. $Co_2MnSi$), while others exhibit perpendicular magnetic anisotropy (e.g. $Co_2FeAl$/MgO(001)). However, until now both properties have not been observed by experiment in a single material. J. Azadani *et al* have predicted that perpendicular anisotropy can be combined with half-metallicity by growing atomic-period superlattices of two different Heusler compounds [1]. We have successfully grown a single-crystal superlattice formed by layers of $Co_2MnAl$ and $Fe_2MnAl$ with periodicity of one to three unit cells using molecular beam epitaxy. X-ray diffraction reciprocal space mapping reveals that the superlattice is compliant to the substrate to at least 20 nm film thickness, sustaining strains from -3.0% (tensile) on MgO(001) to +2.3% (compressive) on GaAs(001). The film strain is accommodated via tetragonal distortion of c/a = 0 .96 to 1.06, respectively. The tetragonal distortion on GaAs(001) contributes to perpendicular magnetic anisotropy, resulting in films exhibiting out-of-plane magnetic easy axes at temperatures below 200K. Films with aluminum content higher than nominal stoichiometry may also help to induce perpendicular magnetization by reducing saturation magnetization, thereby lowering thin-film shape anisotropy. Superlattice structure was verified using electron energy loss spectroscopy in TEM, which shows low interface diffusion of cobalt and iron and high elemental contrast between individual superlattice layers. S pin polarization of >90% near the Fermi level has been measured directly via spin-resolved photoemission spectroscopy. Spin-resolved photoemission spectra suggest that the termination layer near a tunnel barrier interface should be $Co_2MnAl$-like, and may benefit from further composition tuning. This work was supported in part by C-SPIN, one of the six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA. We also acknowledge support from the Vannevar Bush Faculty Fellowship.

[1] J. G. Azadani *et al*. J. Appl. Phys. 119, 043904 (2016).

11:40am **EM+MI+TF-MoM-11 Formation of the Epitaxial MgO/Full-Heusler $Co_2MnSi$ Interface: Oxygen Migration and Elemental Segregation***, **Anthony McFadden**, T Brown-Heft, N Wilson, J Logan, C Palmstrøm,* University of California at Santa Barbara

Magnetic tunnel junctions (MTJs) are an increasingly important emerging technology for both magnetic random access memory (MRAM) and spintronics applications. MTJs utilizing CoFeB magnetic electrodes and MgO tunneling barriers have received considerable interest for use in MRAM as desirable properties including perpendicular magnetic anisotropy, high tunneling magnetoresistance ratio, and current induced switching have been demonstrated. While CoFeB/MgO based MTJs have demonstrated remarkable performance, devices utilizing ferromagnetic Heusler compounds have the potential to surpass CoFeB based technologies due to a much higher predicted spin polarization. In addition, many Heusler candidates have even been predicted to be half-metallic (100% spin polarized at the Fermi-level). Of all predicted half-metals, the full-Heusler $Co_2MnSi$ has received considerable attention as it is quite stable ($\Delta H_F$ = -0.441 eV/atom), has a high Curie temperature ($T_c$=985K), and a large minority-spin energy gap (571 meV). While Heusler based MTJs have the potential to surpass current CoFeB based technology, the spin polarization of Heusler compounds has been shown to be sensitive to atomic ordering, adding an additional challenge to materials growth and integration.

In the present work, the formation of the MgO/$Co_2MnSi$(001) interface has been studied *in-situ* using X-ray photoelectron spectroscopy (XPS). $Co_2MnSi$ layers were grown on Cr-buffered MgO(001) substrates by coevaporation of elemental sources in ultrahigh vacuum while MgO was grown on the $Co_2MnSi$ layers using e-beam evaporation of stoichiometric source material. It was found that partial oxidation of the $Co_2MnSi$ surface was unavoidable during e-beam evaporation of MgO with oxygen bonding preferentially to Mn and Si. Interestingly, oxidation draws Mn and Si to the surface, resulting in an MgO/$Co_2MnSi$ interface with composition significantly different from the unoxidized $Co_2$-MnSi surface. In addition, Mn and Si oxides at the MgO/$Co_2MnSi$ interface were reduced following annealing in UHV with a corresponding migration of oxygen from the interface into the MgO. The results of XPS studies have been correlated with temperature dependent transport measurements of fully epitaxial CoFe/MgO/$Co_2MnSi$ MTJs which were observed to be highly sensitive to post-growth annealing temperature.

## Thin Films Division
## Room 20 - Session TF+EM-MoM
## ALD for Energy Conversion, Storage, and Electrochemical Processes

**Moderator:** Mark Losego, Georgia Institute of Technology

8:20am **TF+EM-MoM-1 Synthesis and Characterization of All Solid-State $SnO_xN_y$/LiPON/Li Batteries***, **David Stewart**, A Pearse, K Gregorczyk, G Rubloff,* University of Maryland, College Park

Atomic layer deposition (ALD) is excellent for depositing conformal thin films on high aspect ratio substrates, and due to the good thickness control and uniformity, ALD allows us to push the limits of thin film batteries. To produce solid-state lithium ion batteries on such substrates new processes for anodes, high-capacity cathodes, and solid-electrolytes must continue to be developed and characterized. Sn and $SnO_2$ have been well studied as alloy/conversion electrodes in the literature, while the properties of $Sn_3N_4$ and $SnO_xN_y$ have yet to be explored in any detail. To study the differences in the electrochemical performance of $SnO_2$, $Sn_3N_4$, and $SnO_xN_y$, an ALD process was developed that allows for highly tunable N/O ratios. In this study tetrakis(dimethylamido)tin (TDMA(Sn)) was used as the metal-organic precursor in combination with remote nitrogen plasma ($^pN$) and $H_2O$ was used to introduce oxygen content. For the pure nitride phase, a broad temperature window was found between 150-250 °C, over which the growth rate per cycle (GPC) was ~ 0.55 Å. While only very short pulse times (< 1 s) were required for saturation of the TDMA(Sn), relatively long $^pN$ exposures (> 20 s) were required for GPC saturation. We then showed that by varying $H_2O$ super cycles the relative concentration of O and N in the film can be controlled between 0% N and 95% N.

To study the electrochemical performance of these materials solid-state half-cells were constructed using $SnO_2$, $Sn_3N_4$, and $SnO_xN_y$ thin films versus thermally evaporated Li. A 100 nm thin film of LiPON was deposited as the solid electrolyte by thermal ALD [1]. This electrolyte layer is thick enough to provide good electrical insulation and thin enough to allow fast ionic diffusion, however when cycled to voltages below 0.4 V vs Li/$Li^+$ the half-cells shorted, possibly due to mechanical breakdown of the LiPON layer from significant volume expansion of the anodes during the alloying reaction with Li. The $Li_2O$ matrix formed from $SnO_2$ is expected to be more stable, but with lower ionic conductivity than the $Li_3N$ matrix formed from $Sn_3N_4$. Galvanostatic intermittent titration and electrochemical impedance spectroscopy were used to analyze the ionic conductivity of the anodes before and after the initial conversion reaction and as a function of N/O ratio. The high capacity of the $SnO_xN_y$ electrodes in combination with the excellent ionic conductivity and mechanical properties of the ALD LiPON makes these films attractive for applications in 3D Li-ion batteries.

[1] A. J. Pearse, T. E. Schmitt, E. J. Fuller, *et. al.* Chemistry of Materials **2017** *29* (8), 3740-3753 DOI: 10.1021/acs.chemmater.7b00805

8:40am **TF+EM-MoM-2 Molecular Layer Deposition for Applications in Lithium-Ion Batteries***, K Van de Kerckhove, F Mattelaer, J Dendooven, **Christophe Detavernier**,* Ghent University, Belgium

Molecular layer deposition (MLD) of hybrid organic-inorganic thin films called *titanicones*, *vanadicones*, *tincones*, and *alucones* was investigated for electrode and solid electrolyte applications in lithium-ion batteries.

The titanicone, vanadicone and tincone films were studied as electrode materials, both as anodes and cathodes. Novel MLD processes were developed for these materials and were based on an alkylamine metal precursor (TDMAT, TEMAV, TDMASn) and glycerol (GL) as the organic reactant [1,2]. Linear and self-limited growth could be achieved for these metalcones in a broad temperature range with temperature-dependant growth rates ranging from 0.2 to 1.3 Å/cycle. Film growth was studied in situ with spectroscopic ellipsometry (SE) and infrared spectroscopy (FTIR). The as-deposited films appeared to be electrochemically inactive in all cases. A post-deposition heat treatment up to 500°C in either inert (helium) or oxidizing (air) atmosphere was able to electrochemically activate the films. X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) measurements showed that all carbon was removed during calcination in air and that the films crystallized. However, annealing in inert atmosphere conserved the carbon content of the film and thus the films remained amorphous. The performance with increasing charging and discharging rate, and cyclability of the heat-treated MLD electrodes was tested against their respective metal oxide references. The He-annealed metalcones emerged from these tests as the best performing electrodes at higher rates and with improved capacity retention and stability during repeated charging and discharging.

The transformation of alucone films, deposited with the TMA and ethylene glycol (EG) or GL process, into porous aluminium oxide was examined. Porous, non-conducting materials are interesting for lithium-ion battery research since they may serve as the matrix template for solid composite electrolytes. Calcination in air and water etching proved to be the most successful methods. For the calcination treatment, a clear relation was found between the ramp rate during both heating and cooling and the resulting porosity of the film. The aging behaviour of the films in ambient atmosphere was also investigated with FTIR and showed that the films deposited with EG decompose in a matter of only a few hours, as opposed to those deposited with GL.

[1] Van de Kerckhove et al., ***Dalton Trans.***, 2016,**45**, 1176-1184.

[2] Van de Kerckhove et al., ***Dalton Trans.***, 2017,**46**, 4542-4553.

9:00am **TF+EM-MoM-3 Engineering Hybrid Thin Film Electrolytes for 3D Lithium-ion Battery Applications*, Ryan Sheil*,** *J Lau,* University of California at Los Angeles*; P Moni,* MIT*; C Choi,* University of California at Los Angeles*; K Jungjohann,* Sandia National Laboratories*; J Yoo,* Los Alamos National Laboratory*; K Gleason,* MIT*; B Dunn, J Chang,* University of California at Los Angeles

3D battery architectures have the potential to meet the power and energy density demands of next generation microelectronic devices. One requirement in the utilization of 3D based electrodes is the incorporation of a solid electrolyte that can be coated pinhole free and conformally on high aspect ratio structures. Lithium aluminosilicate ($Li_xAl_ySi_zO$, LASO), a solid oxide Li-ion conductor, synthesized by atomic layer deposition (ALD) is a promising electrolyte material for 3D battery applications due to its adequate ionic conductivity ($8.2\times10^{-8}$ S/cm) in thin film applications as well as its ability to improve electrode stability. The self-limiting nature of ALD allows precise thickness and composition control when applied to complex metal oxides. Lithium tert-butoxide (LTB), trimethylaluminum (TMA), and tris(tert-butoxy)silanol (TTBS), were precursors used to synthesize LASO by ALD.

In order to further explore potential material properties, ALD deposited LASO was combined with a polymer electrolyte, poly-(tetravinyltetramethylcyclotetrasiloxane) (PV4D4) deposited via initiated chemical vapor deposition (iCVD). The LASO solid electrolyte offers high electrical resistance and chemical stability at the electrochemically active interface, while the pV4D4 solid electrolyte offers improvements in the mechanical integrity of the electrode. A hybrid film consisting of 5 nm LASO and 400 nm PV4D4 demonstrated a room temperature ionic conductivity of $3.4 \times 10^{-7}$ S/cm, showing no significant increase in interfacial resistance. Integration with both 2D and 3D electrodes has shown substantial improvements in cycling and increased coulombic efficiency.

Current research on Li-ion batteries is directed at creating next generation electrode materials. One of the most viable 3D designs is through the use of nanowire electrodes, in which Si and Ge can offer much larger charge capacities (8444 A h $L^{-1}$ for $Li_{15}Si_4$ and 7366 A h $L^{-1}$ for $Li_{15}Ge_4$, respectively) than traditional carbon based anode materials, but suffer large volume expansion upon lithiation. Using an in-situ TEM electrochemical characterization technique, dynamic processes and structural changes are able to be observed during the lithiation/delithiation of a SiGe nanobattery in real time. Preliminary results show that ALD $Li_xAl_ySi_zO$-coated $Si_{0.4}Ge_{0.6}$ alloy nanowire demonstrates lithiation and delithiation with an intact solid state electrolyte layer with ~39% radial expansion observed upon lithiation.

9:20am **TF+EM-MoM-4 Carbon Encapsulated CNT Micropillars for Silicon Lithium Ion Battery Electrodes*, Kevin Laughlin*,** *E Laughlin, R Fan, R Davis, R Vanfleet, J Harb,* Brigham Young University

Here we present work on a hierarchical approach to structuring and encapsulating carbon nanotube (CNT) based carbon monoliths. Prior work has shown silicon has high gravimetric capacity, but increases by ~300%, and forms an unstable solid electrolyte interphase (SEI). High stability and lifetime operation requires nanostructuring of the silicon to alleviate stresses caused by the large expansion of the silicon upon Li alloying, and an encapsulation layer to restrict SEI build up. These CNT structures provide: porous scaffolding for silicon to expand to manage stress on multiple scales, a long conductive path for lithium transfer resulting in tall electrodes, and protection from unstable SEI formation. At high silicon loadings even nanoscale layers of silicon result in stresses large enough to cause mechanical damage to the electrode and encapsulation layer, resulting in lower capacity and cell lifetimes. By patterning the CNT scaffolding, we can contain the stresses caused by lithiation.

9:40am **TF+EM-MoM-5 Porous Oxide Shell on the Supported Gold Nanoparticles Synthesized via Polymer-Templated Atomic Layer Deposition*, Haoming Yan*,** *X Yu, Q Peng,* University of Alabama

Ultra small (≤ 5 nm) metal nanoparticles (USMNPs), especially Au, have attracted increasing attention due to their remarkable catalytic activity and selectivity in many important reactions. However, their catalytic properties are greatly affected by the poor thermal stability and the macro-molecular capping ligand (MCL) layer on their surfaces. Encapsulating the USMNPs with a porous oxide shell (pOXIDE) is a solution for both issues. So far, there has been limited success in generating the pOXIDE shell on the supported USMNP without significantly blocking its active sites. The objective of this work is to demonstrate the MCL layer templated atomic layer deposition (ALD) can be applied to synthesize the pOXIDE shell on the USMNPs to improve their thermal stability while keeping most of the surface active sites on USMNPs for the catalytic reaction.

10:00am **TF+EM-MoM-6 Three-Dimensional Solid State Batteries Grown Via Atomic Layer Deposition*, Alexander Pearse*,** *T Schmitt, D Stewart, E Sahadeo, K Gregorczyk,* University of Maryland, College Park*; K Gerasopoulos,* Johns Hopkins Applied Physics Lab*; G Rubloff,* University of Maryland, College Park

Thin film solid state batteries have multiple attractive properties, including low interfacial impedance, exceptional cycling stability, and intrinsic safety, but have not seen significant implementation because their overall capacity is very low (on the order of 0.1 mAh/cm$^2$). This is a consequence of their growth by physical vapor deposition, which limits them to planar substrates. In this configuration, increasing areal capacity necessarily sacrifices rate performance due to slower ionic diffusion in thicker electrodes. Realizing practical energy or power densities in thin film SSBs will involve the development of entirely new fabrication processes in order to allow the integration of thin film SSBs with 3D substrates, such as micromachined silicon or conductive fabrics. In particular, 3D designs allow the decoupling of capacity and rate performance for area-normalized metrics.

We describe the development and synthesis of a solid state lithium-ion battery film stack grown entirely by atomic layer deposition (ALD), which allows us to successfully integrate solid state energy storage with 3D structures. The entire device is fabricated at temperatures at or below 250C, allowing for compatibility with a broad variety of substrates and processing environments. We utilize a simple electrochemical process for inserting free lithium ions into a crystalline cathode, avoiding the need to integrate lithiation into the ALD growth process itself. The solid electrolyte is a lithium polyphosphazene compound (a variant of LiPON) grown by a 2-precursor thermal process (Pearse et al. Chemistry of Materials 2017). The battery itself is comprised of a $LiV_2O_5 – Sn_xN_y$ couple, providing a reversible capacity of approximately 35 µAh/cm$_2$ µm$_{LVO}$ with an average discharge voltage of 2V. By growing these batteries into micromachined silicon structures with aspect ratios of up to 10, we are able to increase areal capacity by nearly one order of magnitude while simultaneously improving capacity retention at high rates- a type of scaling not possible for planar devices. We also discuss challenges associated with interface chemistry in the ALD growth environment and with patterning highly conformal films, and compare device performance to finite element electrochemical simulation.

10:40am **TF+EM-MoM-8 Systematic Investigation of Geometric Effects in Porous Electrodes for Energy Conversion Reactions*, Julien Bachmann*,** University of Erlangen, Germany **INVITED**

Inexpensive energy conversion devices necessitate novel strategies towards reducing the need for rare functional materials. One such strategy consists in accurately controlling the interface's geometry.

In our work, the pore walls of an anodic nanoporous template are coated with either galvanic deposition or atomic layer deposition (ALD) to obtain structured electrode surfaces that provide the experimentalist with a well-defined, tunable geometry. Indeed, the platform consists of a hexagonally ordered array of metallic or oxidic nanotubes of cylindrical shape, embedded in an inert matrix. The diameter of the tubes can be defined between 20 and 300 nm and their length between 0.5 and 100 µm, approximately. They can be utilized as a model system in which the electrode's specific surface area can be increased and its effect on the electrocatalytic current characterized systematically.

Diffusion-limited electrochemical transformations remain unaffected by changes in the length of the electrode's pores, whereas the steady-state galvanic current density observed for slow multielectron transformations increases linearly with the pore length. In particular, this approach enables us to achieve an increase of the electrochemical water oxidation turnover at neutral pH on iron oxide surfaces by three orders of magnitude. These results highlight a strategy for optimizing electrochemical energy transformation devices which could be generalized: the geometric tuning of catalytically mediocre but abundant and cost-effective material systems.

11:20am **TF+EM-MoM-10 Development of a Reduction-resistant Oxide Electrode for Dynamic Random Access Memory Capacitor***, **CheolJin Cho,** M Noh, W Lee,* Korea Institute of Science and Technology, Republic of Korea*; C An,* Seoul National University, Republic of Korea*; C Kang,* Korea Institute of Science and Technology, Republic of Korea*; C Hwang,* Seoul National University, Republic of Korea*; S Kim,* Korea Institute of Science and Technology, Republic of Korea

Rutile phase $TiO_2/RuO_2$ structures have attracted great interests as a new material system for next-generation dynamic random access memories (DRAM) capacitors because of the high dielectric constant (> 80) of the rutile $TiO_2$. A conducting oxide electrode, $RuO_2$, enables the $TiO_2$ dielectric to be crystallized into a rutile phase at low temperatures (< 300 $^oC$). Since $RuO_2$ has a high work function, it is effective to suppress leakage current by Schottky emission which is a main conduction mechanism of $TiO_2/RuO_2$. However, the $RuO_2$ electrode is easily reduced during the post-annealing under forming gas atmosphere for trap passivation at the gate oxide/Si interface. Subsequently, the dissociated oxygen ions from $RuO_2$ cause problems such as the oxidation of W plug. The oxidation of W plug causes a fatal deterioration in device operation because the W plug acts as a path through which the charges of the capacitor move. Also, physical damage such as cracks will also occur when $RuO_2$(rutile) is reduced to Ru(hexagonal close-packed, HCP). For these reasons, we suggest a $SnO_2$-based electrode, which is a reduction-resistant material, as a new oxide electrode for DRAM capacitors. The reduction reaction of $SnO_2$ is thermodynamically more difficult than that of $RuO_2$. Also, a small amount of Ta ions is incorporated into the $SnO_2$ films to enhance the conductivity of the electrode. The resistivity of $SnO_2$ is reported to reach down to $10^{-4}\Omega\cdot cm$ by Ta doping, which is sufficient for use as an electrode of DRAM capacitor. Furthermore, the Ta-doped $SnO_2$ films are well crystallized into a rutile phase, thereby leading to the formation of rutile $TiO_2$ at a low growth temperature (< 270 $^oC$). Therefore, we demonstrate that Ta-doped $SnO_2$ would be a promising candidate for the electrodes for next-generation DRAM capacitors.

## Spectroscopic Ellipsometry Focus Topic
## Room 9 - Session EL+AS+EM-MoA
### Spectroscopic Ellipsometry: Novel Applications and Theoretical Approaches

**Moderator:** Maria Losurdo, University Bari

1:40pm **EL+AS+EM-MoA-1 Temperature Dependent Mueller Matrix Measurements of Magnetised Ni near the Curie Temperature***, **Farzin Abadizaman**, S Zollner,* New Mexico State University

The temperature dependence of the optical constants of the magnetized bulk Ni demonstrates an anomaly near the Curie temperature. We investigate this anomaly by taking a measurement of the temperature dependent Mueller Matrix (MM). Using spectroscopic ellipsometry at an energy 1.96 eV, the MM measurement was taken from 350 K to 500 K with 10 K steps, and from 500 K to 670 K with 1 K steps, and from 670 K to 730 K with 10 K steps.

In order to distinguish the anisotropic properties of the magnetized Ni from the windows effects, three samples (Ge, Ni, and SiO-$_2$ on Si) were measured inside the cryostat in the energy range from 1 eV to 5 eV with 0.1 eV steps. The results show that the anisotropic elements of the MM behave in the same fashion for all samples, except for element M$_{24}$-,which depends on the sample.

The MM data of magnetized Ni indicate very small changes in the anisotropic portion of the MM compared to the windows effect. The authors believe that these changes are due to the magneto-optical Kerr effect. However, since a rotating-analyzer ellipsometer was used, the last row of the MM is absent and a complete MM measurement needs to be performed to find the magneto-optical Kerr effect in the other anisotropic elements too.

However, very large decreases in the isotropic MM elements were found near the Curie temperature. This means, the changes in optical constants near T--c-- are due to the on-diagonal Drude part of the dielectric tensor, which can be explained by s- to d-band electron-phonon scattering above and below $T_c$. These changes are absent when decreasing the temperature and for unmagnetized Ni.

2:00pm **EL+AS+EM-MoA-2 Ellipsometry Based Observation of Material Ordering Process in Holography***, **Hao Jiang**, H Peng, Y Liao, S Liu,* Huazhong University of Science and Technology, China

Ordered materials with superior performance have been constantly pursued. Nevertheless, the direct, precise and non-destructive observation of the ordering process, which is especially critical for continuous manufacturing, remains a formidable challenge. Herein, we introduce Mueller matrix ellipsometry (MME) as a nondestructive method to quantitatively observe the material ordering process during holography. This non-destructive observation directly offers the exact width, refractive index, nanoparticle weight fraction and volume fraction in each constructive (bright) or destructive (dark) interference area, which is impossible to be implemented using other existing techniques. Meanwhile, the width of dark region is observed to decrease while the width of bright region increases with an augmentation of the holographic recording time, distinct from previous assumption. More importantly, an apparent diffusion coefficient of $1.3\times10^{-15}$ $m^2$ $s^{-1}$ is determined on the basis of recording time-dependent grating structure observation, which is 3 orders of magnitude lower than the Stokes-Einstein prediction. The distinct diffusion coefficient is regarded to be the result of competition between the forth diffusion driven by the chemical reaction and backward diffusion arising from nanoparticle concentration gradient. This novel protocol is envisioned to pave the way for precisely and non-destructively understanding the ordered structure formation in electrics, photonics, photovoltaics, biomaterials and other disciplines.

2:20pm **EL+AS+EM-MoA-3 Coherence in Polarimetry and Ellipsometry: Synthesizing Mueller Matrices in an Ellipsometer***, **Oriol Arteaga**,* Departament de Física Aplicada, Universitat de Barcelona, Spain **INVITED**

Interference phenomena are ubiquitous in optics and are the basis of the industry behind thin film optical coatings or thin film thickness measurements with ellipsometry. The interference of polarized beams was experimentally understood in 1819 when Arago and Fresnel derived the four laws governing the interference of polarized light. While spectroscopic ellipsometry provides information based on the position and number of interference oscillations in thin films, typically one has no macroscopic control of the beams that coherently superpose.

In this work we present a polarimetric analysis of an analogue of Young's double slit experiment that allows merging beams in a well-controlled manner. The experiment is analyzed with a new formalism that is useful to describe optical coherence and polarization and that shows that the superposition of two macroscopically distinguishable beams can be an effective method to experimentally synthesize Mueller matrices with on-demand polarization properties. This offers the opportunity of working with "synthesized" optical elements that behave just like "real" ones. We will discuss how this method can have a practical application in the construction of ellipsometers or polarimeters.

3:00pm **EL+AS+EM-MoA-5 Femtosecond Spectroscopic Ellipsometry on Optoelectronic Materials and Photonic Structures***, **Mateusz Rebarz**, S Espinoza,* ELI Beamlines - Czech Academy of Science, Czech Republic*; S Richter, O Herrfurth, R Schmidt-Grund,* Universität Leipzig, Germany*; J Andreasson,* Chalmers University of Technology, Sweden*; S Zollner,* New Mexico State University

The ongoing progress in miniaturization and operational rates of electronic and optoelectronic devices obliges materials scientists to deeply understand the dynamics of the carriers upon external electromagnetic stimulus in very short time scale. Some phenomena such as scattering of electrons and phonons as well as recombination processes can be as short as tens of femtoseconds. All these processes affect the temporal and local dielectric constants and determine many operational parameters of the devices. In this work, we report on recent progress in developing a spectroscopic ellipsometer for characterization of ultrafast dynamic changes of dielectric properties in materials and photonic structures technologically relevant in optoelectronics. Our time-resolved ellipsometer is based on pump-probe technique and offers monitoring the time evolution of the dielectric properties in range 0-5 ns with time resolution ~100 fs in broadband spectral range (340-750 nm).

We present here the results of the measurements performed on Ge samples in comparison with theoretical predictions. Ultrafast phenomena such as excitation, relaxation and diffusion of charge carriers, band-gap renormalization and excitons screening will be discussed. In addition we report on the first data obtained from a ZnO-based planar microcavity especially on the temporal evolution of the microcavity modes. The time evolution of the ellipsometric parameters in the spectral range around the exciton-polariton mode will be discussed. We observed that such modes disappear upon the excitation, possibly due to screening of the excitons and re-appear after a few hundreds of femtoseconds as blueshifted modes. The investigation of the short-time dynamics of such modes can stimulate new theoretical approaches for the description of exciton-polariton systems.

3:20pm **EL+AS+EM-MoA-6 Temperature Dependence of the Dielectric Function and Interband Critical Points of Bulk Germanium***, **Carola Emminger**, N Samarasingha, F Abadizaman, N Fernando, S Zollner,* New Mexico State University

Exploration of the optical properties of bulk germanium (Ge) is necessary for the advancement of Ge technology. In fact, many of the Ge applications depend on the dielectric function (ε), which is directly related to the electronic band structure. Here we investigate the effect of temperature on the optical properties and interband critical points (CPs), primarily the $E_0$ and $E_0+\Delta_0$ critical points of bulk Ge in the temperature range from 10 to 738 K using spectroscopic ellipsometry at 70° angle of incidence. The data was taken in two parts, in the near IR region and in the UV region, which provides data from 0.5 to 6.2 eV. The low temperature environment was created in a UHV cryostat with liquid helium and nitrogen as cryogens. To reduce the thickness of the native $GeO_2$ layer, the Ge sample was cleaned using ultra-pure water, isopropanol, an ultrasonic bath and ozone cleaning. It was possible to reduce the oxide thickness to about 11 Å at room temperature.

The authors used a two-phase model ($GeO_2$ layer/Ge substrate) and a parametric oscillator model with a set of adjustable parameters to extract the real and imaginary parts of the complex dielectric function of the bulk Ge for the whole temperature range. To investigate this temperature dependence of the CP parameters (threshold energy, broadening and phase angle) further, we also compared the second derivative $d^2\varepsilon/d^2\omega$ of the dielectric function with analytical line shapes.

The temperature has a significant influence on both the real and imaginary parts of the complex dielectric function of bulk Ge. This temperature dependent ε can be explained by a Bose-Einstein occupation factor. Due to the electron-phonon interaction, we find a temperature dependent red shift (shift to lower energies) of the $E_0$ and $E_0+\Delta_0$ critical point energies. The temperature independent spin orbit splitting $\Delta_0$ is found to be 286 meV. A similar effect has been seen in the $E_1$, $E_1+\Delta_1$, $E_0'$, and $E_2$ CP energies. These CPs are broadened and shifted to the lower energies with increasing temperature.

4:00pm **EL+AS+EM-MoA-8 VUV Magneto-Optical Transient Ellipsometer*, Shirly Espinoza,*** *J Andreasson,* Institute of Physics ASCR, Czech Republic

This talk is about the ELIps instrument, an instrument that combines three advanced techniques of ellipsometry: VUV ellipsometry, Transient (Pump-probe) ellipsometry, and Magneto-optical ellipsometry [1].

The ELIps instrument allows users to work in a very wide range of energies from 1 eV to 40 eV. For measurements in the 1 eV to 6.5 eV range, it uses a transmission polarizer and analyzer combination. Meanwhile, for measurements in the 6.5–40 eV range, it uses a triple-reflection polarizer and analyzer combination. All the components are contained within a single UHV chamber designed with several additional ports to support future upgrades. For time resolved measurements in the VUV range the instrument will be used together with a high intensity High Harmonics Generation (HHG) source.

Time-resolved transient measurements of the optical properties of materials can be performed in the range of a few femtoseconds to nanoseconds. Initial experiments with transient absorption and transient ellipsometry in the NIR-UV range is being performed on proton-conducting materials for solid oxide fuel cell applications.

Additionally, ELIps is equipped with a Helmholtz coil, which allows the studies of the transverse magneto-optical Kerr effect on the sample, and with a cryostat for measurements at different temperatures.

Where is this instrument located? ELIps is in Prague, Czech Republic, at the European Extreme Light Infrastructure Beamlines (ELI Beamlines), a user facility project that will hold some of the most intense lasers in the world. It will open to the public on January 2018.

References

[1] S. Espinoza, G. Neuber, C. D. Brooks, B. Besner, M. Hashemi, M. Rübhausen and J. Andreasson. 2017. User oriented end-station on VUV pump-probe magneto-optical ellipsometry at ELI beamlines. *Applied Surface Science*. Published online. doi:10.1016/j.apsusc.2017.02.005

Acknowledgements

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4:20pm **EL+AS+EM-MoA-9 Infrared Ellipsometric Spectroscopy of $Hg_{1-x}Cd_xTe$ Bulk Samples*, Yanqing Gao,*** Shanghai Institute of Technical Physics, Chinese Academy of Sciences, China

**The infrared spectroscopic ellipsometry of $Hg_{1-x}Cd_xTe$ ($x$=0.195~0.37) bulk samples with different compositions were meaured. The refractive index n and extinction coefficient k were obtained. An obvious refractive index enhancement effect was observed in the refractive index spectra for each composition. The energy position of the maximal refractive index value equals approximately that of the band gap. With the decrease of the component, the refractive index increased and the peak position shifted to the low energy direction, which consistented with the absorption edge. The refractive index n at Eg changed linearly with the composition $x$.**

4:40pm **EL+AS+EM-MoA-10 Infrared Ellipsometry Study of the Photo-generated Charge Carriers at the (001) and (110) Surfaces of $SrTiO_3$ Crystals and the Interface of Corresponding $LaAlO_3/SrTiO_3$ Heterostructures*, Meghdad Yazdi-Rizi,*** *P Marsik, B Mallett,* University of Fribourg, Switzerland*; K Sen, A Cerreta,* University of Fribourg*; A Dubroka,* Masaryk University*; M Scigaj, F Sánchez, G Herranz,* Institut de Ciència de Materials de Barcelona*; C Bernhard,* University of Fribourg, Switzerland

With infrared (IR) ellipsometry and DC resistance measurements we investigated the photo-doping at the (001) and (110) surfaces of $SrTiO_3$ (STO) single crystals and at the corresponding interfaces of $LaAlO_3/SrTiO_3$ (LAO/STO) heterostructures. In the bare STO crystals we find that the photo-generated charge carriers, which accumulate near the (001) surface, have a similar depth profile and sheet carrier concentration as the confined electrons that were previously observed in LAO/STO (001) heterostructures. A large fraction of these photo-generated charge carriers persist at low temperature at the STO (001) surface even after the UV light has been switched off again. These persistent charge carriers seem to originate from oxygen vacancies that are trapped at the structural domain boundaries which develop below the so-called antiferrodistortive transition at $T^*$ = 105 K. This is most evident from a corresponding photo-doping study of the DC transport in STO (110) crystals for which the concentration of these domain boundaries can be modified by applying a weak uniaxial stress. The oxygen vacancies and their trapping by defects are also the source of the electrons that are confined to the interface of LAO/STO (110) heterostructures which likely do not have a polar discontinuity as in LAO/STO (001). In the former, the trapping and clustering of the oxygen vacancies also has a strong influence on the anisotropy of the charge carrier mobility. We show that this anisotropy can be readily varied and even inverted by various means, such as a gentle thermal treatment, UV irradiation, or even a weak uniaxial stress. Our experiments suggest that extended defects, which develop over long time periods (of weeks to months), can strongly influence the response of the confined charge carriers at the LAO/STO (110) interface.

## Electronic Materials and Photonics Division
## Room 14 - Session EM-MoA

### Novel Materials and Devices for Electronics

**Moderators:** Shalini Gupta, Northrop Grumman ES, Rehan Kapadia, University of Southern California

1:40pm **EM-MoA-1 2D Materials for Advanced Devices: Integration Challenges and Opportunities*, Robert M. Wallace,*** University of Texas at Dallas **INVITED**

The size reduction and economics of integrated circuits, captured since the 1960's in the form of Moore's Law, continues to be challenged. Challenges include addressing aspects associated with truly atomic dimensions, while the cost of manufacturing is increasing such that only 3 or 4 companies can afford leading edge capabilities. To address some of the materials physical limitations, "2D materials" such as graphene, phosphorene, h-BN, and transition metal dichalcogenides have captured the imagination of the electronics research community for advanced applications in nanoelectronics and optoelectronics. Among 2D materials "beyond graphene," some exhibit semiconducting behavior, such as transition-metal dichalcogenides (TMDs), and present useful bandgap properties for applications even at the single atomic layer level. Examples include "$MX_2$", where M = Mo, W, Sn, Hf, Zr and X = S, Se and Te

Integration of these materials with semiconductor industrial fabrication processes presents a number of challenges. For example, several synthesis methods have been employed to study 2D material thin film properties including mechanical/liquid exfoliation, chemical bath deposition, vapor phase deposition, and molecular beam epitaxy (MBE). From a manufacturability and cost perspective, vapor phase (including chemical and atomic layer) deposition are the subject of intense research activity in the electronics industry, while MBE methods facilitate the research of large thin films in advance of precursor development for CVD and ALD.

This presentation will examine the state-of-the-art of these materials in view of our research on 2D semiconductors, and the challenges and opportunities they present for electronic and optoelectronic applications. [1]

This work is supported in part by: (i) the SWAN Center, a SRC center sponsored by the Nanoelectronics Research Initiative and NIST, (ii) the Center for Low Energy Systems Technology (LEAST), one of six centers supported by the STARnet phase of the Focus Center Research Program (FCRP), a Semiconductor Research Corporation program sponsored by MARCO and DARPA, (iii) the US/Ireland R&D Partnership (UNITE) under the NSF award ECCS-1407765, and (iv) the Erik Jonsson Distinguished Chair in the Erik Jonson School of Engineering and Computer Science at the University of Texas at Dallas.

1. S. J. McDonnell and R.M.Wallace, "Critical Review: Atomically-Thin Layered Films for Device Applications based upon 2D TMDC Materials", Thin Solid Films, 616, 482-501 (2016).

3:00pm **EM-MoA-5 Enhancement-mode AlGaN/GaN HEMTs Enabled by ALD ZrO2 Gate Dielectrics***, **Charles Eddy, Jr.**, V Wheeler,* U.S. Naval Research Laboratory*; D Shahin,* University of Maryland*; T Anderson, M Tadjer, A Koehler, K Hobart,* U.S. Naval Research Laboratory*; A Christou,* University of Maryland*; F Kub,* U.S. Naval Research Laboratory

If power switches based on gallium nitride (GaN) transistors are to achieve widespread adoption, then reliable enhancement-mode (normally-off) operation must be demonstrated. The most advanced GaN transistor, the high electron mobility transistor (HEMT), is naturally a depletion-mode (normally-on) device and is finding rapid adoption in RF applications requiring high power and efficiency. To extend these performance benefits to power switches requires fully depleting the two-dimensional electron gas below the gate in absence of a gate bias. This is often achieved by recess etching the AlGaN barrier under the gate. However, to ensure low gate leakage in such a device further requires a reliable gate dielectric on this recessed surface. Here we report on the development and application of ALD deposited $ZrO_2$ gate dielectrics on recessed etched GaN surfaces. First, a thorough investigation of recessed surface pretreatments is conducted. Then, ALD is used to deposit $ZrO_2$ dielectrics on these surfaces using two precursors – zirconium (IV) tertbutoxide and tetrakis(dimethylamino)zirconium. Through careful variations in ALD growth conditions and precursor selection, we demonstrate the ability to achieve a record positive shift in the threshold voltage for a HEMT of up to +3.99V [1] and low gate leakage currents (5 orders of magnitude lower than reference HEMTs) under on-state conditions (Vgs= +10V and Vds= +20V). These promising early results have been followed by studies of traps in these device structures using a previously established method [2]. Details of recessed surface preparation and trap behavior will be presented.

[1] T.J. Anderson et al., Appl. Phys. Express 9, 071003 (2016).

[2] J. Joh and J. A. del Alamo, IEEE Trans. Electron. Dev. 58, 132 (2011).

3:20pm **EM-MoA-6 Interface Engineering with $Al_2O_3$-$HfO_2$ Nanolaminate Gate oxides on Silicon Germanium***, **Mahmut Kavrik**,* University of California at San Diego*; K Tang,* Stanford University*; E Thomson, J Cheng, A Kummel,* University of California at San Diego

Silicon Germanium (SiGe) alloys are promising alternative for silicon in semiconductor industry due to their tunable bandgap and carrier mobility through variation in composition. However, replacement of Si with SiGe requires a new class of high-k dielectric gate oxides with low leakage current for CMOS processing. Germanium content in semiconductor induces new interface defects due to its bonding with oxygen; GeOx is soluble in water and also can out diffuse into the gate oxide. $Al_2O_3$ and $HfO_2$ oxides were incorporated into nanolaminate stacks on the SiGe by Atomic Layer Deposition (ALD). $Al_2O_3$ was deposited with organic precursor trimethylaluminum (TMA) and $H_2O$ on SiGe at 250C after HF and sulfur surface treatments. Sulfur treatment forms Ge-S and Ge-S-Ge bonds and prevents GeOx formation. Subsequently, HfO2 oxide layers were grown with organic precursor Tetrakis(dimethylamido) hafnium(TDMAH) and $H_2O$ at 250C. $Al_2O_3$-$HfO_2$ nanolaminates were terminated with one layer of $Al_2O_3$ to protect oxide from gate metal damage. MOSCAP studies showed low Dit with hig Cox with Nanolaminate structure.

4:00pm **EM-MoA-8 Encapsulation of AlGaN/GaN High Electron Mobility Transistor based Hydrogen Sensor for Humid Ambient Sensing Application***, S Jung, H Kim,* Dankook University*; K Baik,* Hongik University*; F Ren, S Pearton,* University of Florida*; **Soohwan Jang**,* Dankook University

Hydrogen is environmentally friendly alternative energy source and carrier for automotive and fuel cell applications as well as in many industrial processes. Hydrogen gas is colorless, odorless, extremely reactive with oxygen, and has very low ignition energy. Especially, leaking gas from pressurized container may elevate its temperature, and induce spontaneous flammable ignition due to its negative Joule-Thomson coefficient. Therefore, hydrogen gas sensing systems are essential in various hydrogen related applications. GaN based material system is well-suited to hydrogen sensing because of its wide bandgap for high temperature operation, and mechanical and chemical robustness for device reliability. Many types of devices based on the GaN, including Schottky diodes, metal oxide semiconductor diodes, GaN nanowires and AlGaN/GaN high electron mobility transistors have been developed for fast and sensitive detection of hydrogen. Among them, AlGaN/GaN HEMTs with a 2 dimensional electron gas (2DEG) channel induced by piezoelectric and spontaneous polarization between the AlGaN and GaN layers showed high sensitivity to change in surface charge created by catalytic reaction of Pt or Pd with hydrogen. With 30 % Al concentration in AlGaN layer, 5~10 times higher electron densities in 2DEG are obtained compared to typical GaAs or InP HEMTs, which induces higher current and better sensitivity of the device. However, one of issues with semiconductor based hydrogen sensors is the fact that their sensitivity is significantly degraded in the presence of humidity or water. Water molecules block the catalytically active sites of sensing material, and results in the significant reduction in hydrogen detection signal. By employing encapsulation layer which prevents water molecules from adsorbing on the active sites of the sensor while selectively allowing penetration of hydrogen molecules, this issue can be solved. In this paper, we demonstrate that the device encapsulated with a moisture barrier does not suffer from any significant change in hydrogen detection sensitivity in the presence of moisture and that the devices can be repeatedly cycled to temperatures up to 300°C without any change in characteristics. Also, the device did not respond to the other gases including $CH_4$, CO, $NO_2$, $CO_2$, and $O_2$.

4:20pm **EM-MoA-9 Work Function Measurements of Metal Gate - TiAlC by Ultraviolet Photoelectron Spectroscopy***, **Yibin Zhang**, H Wang, D Shao, Y Liang,* GlobalFoundries Inc

In order to obtain high performance and low power in integrated circuits (IC), feature sizes continue to shrink and new materials are being developed. One major challenge is finding a metal gate electrode with the appropriate work function when paired with a gate oxide. Titanium-Aluminum-Carbide (TiAlC) films deposited by Atomic Layer Deposition (ALD) were introduced in the semiconductor industry in the 22nm and beyond FINFET technology node. TiAlC can provide the necessary work function and ALD offers better thickness control, uniformity and conformity compared to Plasma Vapor Deposition (PVD). Electrical measurements are typically used to measure a film's work function. However, in an IC manufacturing environment this type of measurements can be performed only after several processing steps following the TiAlC deposition. It is often difficult and not cost effective to "rework" the affected wafers resulting in the loss of both product and time. Thus, it is important to monitor the work function during manufacturing. X-ray Photoelectron Spectroscopy (XPS) is used for in-line monitoring of the film composition and thickness, but it cannot directly measure the work function of TiAlC. In this work we demonstrate that Ultraviolet Photoelectron Spectroscopy (UPS) can provide work function measurements directly after the film deposition, to more effectively control the TiAlC ALD process parameters and resulting film properties. In addition, X-ray reflectivity (XRR) and X-ray diffraction (XRD) were used to investigate TiAlC film's density and crystallinity.

4:40pm **EM-MoA-10 Nitride Based Avalanche Photodiode Detector Structures for Nuclear Detection Applications***, **Vincent Woods**, L Hubbard, L Campbell,* Pacific Northwest National Laboratory*; N Dietz,* Georgia State University*; Z Sitar,* North Carolina State University **INVITED**

Group III-N avalanche photodiodes (APD) offer tailorable UV sensitivity and selectivity not currently available for scintillated light detectors. Materials growth challenges continue to hamper the development and implementation of UV III-N detectors. This presentation details the efforts at Pacific Northwest National Laboratory in collaboration with North Carolina State University and Georgia State University to develop device structures and fabrication processes Group III-N APDs. The focus of these efforts is to produce nitride photomultiplier (NPM) devices similar to a silicon photomultiplier (SiPM). Compared to traditional photomultiplier tubes (PMTs), the NPMs can be smaller, more rugged, consume less power than PMTs, and have lower dark currents than SiPMs for UV light detection.

The large bandgap of III-N systems allows for UV photo-detection that is solar blind resistant to ambient stray light. Unlike silicon, the bandgap and associated dark current in the III-N system can be tuned by changing the composition of the $Al_xGa_{1-x}N$ materials system. A direct advantage of the III-N APDs over SiPMs and PMTs is the matching of the device (by matching the band gap) to a scintillator.

Conventional radiation detection relies on the use of dyes to wavelength shift the scintillated light to match the PMT or SiPM. Tailoring the APD to the scintillator allows for increased resolution of scintillated light without broadening/attenuation from dye interactions. A tailorable APD also allows for exploration of scintillating materials which cannot be dye matched to a SiPM or PMT. The tailorable III-N system opens up new avenues in radiation detection. Research into the selection of appropriate scintillator materials and compositional requirements of the Nitride-based APD structures will be presented. In addition to the materials characterization, optoelectronic modeling aimed towards efficient APD operation will be shown.

The progress in the growth of nitride heterostructures in both Al-rich and Ga-rich Al-GaN materials systems will be presented along with detailed materials characterization. This project is developing the materials capability to tailor III-N APDs to match scintillated light. The development of materials knowledge and capability will enable tailorable III-N APDs for direct matching to UV scintillated light, a significant improvement over current technology.

## Magnetic Interfaces and Nanostructures Division
## Room 11 - Session MI+BI+EM+SA-MoA

## Role of Chirality in Spin Transport and Magnetism

**Moderators:** Greg Szulczewski, The University of Alabama, Hendrik Ohldag, SLAC National Accelerator Laboratory

1:40pm **MI+BI+EM+SA-MoA-1 Spin Transport and Polarization in Chiral Molecules: Theory and Possible Applications***, **Karen Michaeli,*** Weizmann Institute of Science, Israel **INVITED**

The functionality of many biological systems depends on reliable electron transfer. Unlike artificial electric circuits, electron transport in nature is realized via insulating chiral (i.e., parity-symmetry breaking) molecules. Recent experiments have revealed that transport through such molecules strongly depends on the electron's spin relative to the propagation direction. In the talk I will introduce the mechanism behind this phenomenon, which has been dubbed chiral induced spin selectivity (CISS). The discovery of the CISS effect has raised important questions about the role of spin in biological processes more generally, and suggests the possibility of a new class of organic-based nanoscale devices. I will discuss some of the key developments regarding spin selectivity; I will present new questions that arise from these results and offer ideas for their resolution.

2:20pm **MI+BI+EM+SA-MoA-3 Enantio-sensitive Charge Transfer in Adsorbed Chiral Molecules Probed with X Ray Circular Dichroism***, F Luque,* Universidad Autónoma de Madrid, Spain*; I Kowalik,* Polish Academy of Sciences, Poland*; M Niño,* IMDEA-Nanoscience, Spain*; D Arvanitis,* Uppsala University, Sweden*; **Juan José de Miguel,*** Universidad Autónoma de Madrid, Spain

Recent studies have shown how layers of purely organic, chiral molecules can induce the appearance of strong spin polarization in initially unpolarized electron currents. [1] Furthermore, spin-polarized photoemission experiments comparing adsorbed films of opposite enantiomers of the same chiral molecule have revealed that they can display different behavior, producing spin polarization along different directions in space instead of simply changing its sign. [2]

In this study enantio-pure ultrathin films of chiral 1,2-diphenyl-1,2-ethanediol (DPED) have been deposited on Cu(100) at 100 K and studied at the MAX-lab synchrotron in Lund, Sweden, using circularly polarized x ray absorption (XAS) at the carbon K edge. XAS excites element-specific core electrons to empty levels in the ground state thus probing the molecule's electronic configuration. The different features present in the absorption spectra have been identified and assigned to specific electronic transitions. The comparison of absorption spectra taken with photons of opposite helicity shows a surprisingly strong dichroism localized at transitions into empty molecular orbitals with $\pi$ character. Theoretical modeling of the spectra reveals that this response is associated to the charge transferred between the Cu substrate and the adsorbed molecules. This charge is found to be polarized in orbital momentum, and the direction of the polarization is different for the two enantiomers studied: (R,R)–DPED and (S,S)–DPED. These findings indicate that chiral organic layers can play an important role in the emerging field of molecular orbitronics.

[1] B. Göhler V. Hamelbeck, T. Z. Markus, M. Kettner, G. F. Hanne, Z. Vager, R. Naaman, and H. Zacharias, Science **331**, 894 (2011).

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2:40pm **MI+BI+EM+SA-MoA-4 Evolving of Soliton Phase in Exfoliated 2D Cr$_{1/3}$NbS$_2$ Nanolayers***, S Tang,* Oak Ridge National Laboratory and Central South University, China, PR China*; J Yi, R Fishman, S Okamoto, Q Zou,* Oak Ridge National Laboratory*; D Mandrus,* University of Tennessee*; **Zheng Gai,*** Oak Ridge National Laboratory

Cr1/3NbS2 is an emergent quasi-2D material that has recently been attracting wide attentions. Cr1/3NbS2 has both chiral helimagnetic behavior and broken inversion symmetry of Cr atoms, the two necessary conditions for creating Dzyaloshinskii–Moriya interaction in skyrmion. Bulk studies show that a nonlinear periodic magnetic state called a soliton lattice exists in the material. By applying microexfoliation techniques, we successfully prepared thin layers of Cr1/3NbS2 with various thickness from single crystal. When the thickness of Cr1/3NbS2 layer falls into the range around the pitch of its helimagnetic state, kinks of field dependent magnetization start to evolve. The new phase is studied experimentally and theoretically. This research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

3:00pm **MI+BI+EM+SA-MoA-5 Tailoring the Chirality of Domain Walls via Interface Modification***, **Arantzazu Mascaraque**, S Ruiz-Gomez, M Gonzalez Barrio, L Perez,* Universidad Complutense de Madrid, Spain*; G Chen, A Schmid,* Lawrence Berkeley National Laboratory*; E Michel,* Universidad Autonoma de Madrid, Spain

The possibility of manipulating magnetic domain walls (DWs) without the intervention of magnetic fields has interest for a wide variety of applications, such as spintronic devices [1]. Applying an electric current to a ferromagnet creates a force that drives the DWs in the direction of the electron motion, the so-called Spin Transfer Torque. However, this effect is weak and high current densities are needed. Recently, it has been discovered that spin accumulation at the edges of a current-carrying non-magnetic material due to the Spin Hall Effect (SHE), can exert a torque on the magnetization of a neighboring magnetic layer [2]. The torque induced by SHE depends on the chirality of the DW and, as most ferromagnetic materials lack a well-defined chirality, the device applications are limited. However, the presence of surfaces and interfaces removes the point-inversion symmetry, giving rise to an additional interaction, the Dzyaloshinskii–Moriya interaction (DMI) that lifts the left-right degeneracy through spin-orbit coupling [3].

In this work, we have modified the interface between the substrate and a non-chiral magnetic layer, in order to investigate in which way DW chirality can be induced and stabilized in the magnetic layer. The experiments were done using the SPLEEM instrument of the Lawrence Berkeley National Laboratory. This microscope can map independently and in real space the three magnetic components of the spin structures. The magnetic system was a (Ni/Co)n multilayer epitaxially grown on Cu(111). It is well known that magnetic films grown on Cu(111) do not exhibit homo-chiral DWs [4]. We have found that this behavior can be changed by modifying the interface. After introducing a thin metal layer (suitable to induce a high DMI) between the substrate and the magnetic layer, we have found relevant changes in the chirality of the DWs of the magnetic layer. Our results demonstrate that the buffer layer influences the spin texture, which evolves from non-chiral Bloch to homo-chiral Néel DWs.

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3:20pm **MI+BI+EM+SA-MoA-6 Spin Transport in an Electron Conducting Polymer***, **Greg Szulczewski**, T Sutch, M Lockart, H Chen, P Rupar, M Bowman,* The University of Alabama

We report results from an electron spin resonance (ESR) study to probe the spin-dynamics in the conducting polymer poly {[ N, N9 -bis(2-octyldodecyl)-naphthalene-1,4,5,8-bis(dicarboximide)-2,6-diyl]-alt-5,5 9 -(2,2 9 -bithiophene)} or P(NDI2OD-T2). Chemical reduction of the polymer was achieved by using cobaltacene, which introduces unpaired electrons into the polymer. Continuous wave ESR measurements were done on frozen solutions and thin films over the temperature range of 77 to 300 K. Narrow ESR peaks with broad tails were observed, suggesting strong one-dimensional anisotropic conduction. Electron nuclear double resonance spectroscopy was used to analyze the hyperfine coupling of the frozen solutions. The results indicate a proton hyperfine coupling of 1.5 MHz, which suggests the spins are delocalized over several monomer units. Electron spin echo envelope modulation spectroscopy was measured from 6 to 90 K to investigate the spatial distribution of nuclear spins in the environment of the unpaired electrons spins. The measurements show that spin relaxation increases rapidly when the temperature in increases from 6 to 90 K. A kinetic model that accounts for the spin-dynamics will be presented.

4:00pm **MI+BI+EM+SA-MoA-8 Utilizing the Chiral induced Spin Selectivity Effect to Achieve Simple Spintronics Devices***, Yossi Paltiel,* The Hebrew University of Jerusalem, Israel **INVITED**

With the increasing demand for miniaturization, nano-structures are likely to become the primary components of future integrated circuits. Different approaches are being pursued towards achieving efficient electronics, among which are spin electronics devices (spintronics) [1]. In principle, the application of spintronics should result in reducing the power consumption of electronic devices.

A new, promising, effective approach for spintronics has emerged using spin selectivity in electron transport through chiral molecules, termed Chiral-Induced Spin Selectivity (CISS) [2]. Recently, by utilizing this effect we demonstrated a magnet-less magnetic memory [3,4]. Also we achieve local spin-based magnetization generated optically at ambient temperatures [5,6]. The locality is realized by selective adsorption of the organic molecules and the nano particles [7]. Lastly we have been able to show chiral proximity induced magnetization on the surface of ferromagnetic and superconducting materials. The magnetization is generated without driving current or optically exciting the system [8,9].

In the talk I will give a short introduction about spintronics and the CISS effect. Then I will present ways achieve simple spintronics devices utilizing the effect.

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[8] H. Alpern, E. Katzir, S. Yochelis, Y. Paltiel, and O. Millo; New J. Phys. 18 113048 (2016).

[9] O. Ben Dor, S. Yochelis, A. Radko, K. Vankayala, E. Capua, A. Capua, S.-H. Yang, L. T. Baczewski, S. S. P. Parkin, R. Naaman, and Y. Paltiel; *Nature Communications*, **8** 14567 (2017).

4:40pm **MI+BI+EM+SA-MoA-10 Magnetic Nano Platelets based Spin Memory Device Operating at Ambient Temperatures***, Guy Koplovitz,* The Hebrew University of Jerusalem*; Y Paltiel,* The Hebrew University of Jerusalem, Israel

There is an increasing demand for realizing a simple Si based universal memory device working at ambient temperatures. In principle non-volatile magnetic memory could operate at low power consumption and high frequencies. However, in order to compete with existing memory technology, size reduction and simplification of the used material systems are essential. In our work we use the Chiral Induced Spin Selectivity (CISS) effect along with 30-50nm Ferro-Magnetic Nano Platelets (FMNPs) in order to realize a simple magnetic memory device. The vertical memory is Si compatible, easy to fabricate and in principle can be scaled down to a single nano particle size. Results show clear dual magnetization behavior with threefold enhancement between the one and zero states. The magnetization of the device is accompanied with large avalanche like noise that we ascribe to the redistribution of current densities due to spin accumulation inducing coupling effects between the different nano platelets.

5:00pm **MI+BI+EM+SA-MoA-11 Magnetization Switching in Ferromagnets by Adsorbed Chiral Molecules without Current or External Magnetic Field***, Oren Ben Dor*[1,2]*,* The Hebrew University of Jerusalem, Israel

Ferromagnets are commonly magnetized by either external magnetic fields or spin polarized currents. The manipulation of magnetization by spin-current occurs through the spin-transfer-torque effect, which is applied, for example, in modern magnetoresistive random access memory. However, the current density required for the spin-transfer torque is of the order of $1\times10^{6}$ $A\cdot cm^{-2}$, or about $1\times10^{25}$ $electrons\cdot sec^{-1}\cdot cm^{-2}$. This relatively high current density significantly affects the devices' structure and performance. Here, we present a new effect – that of magnetization switching of ferromagnetic thin layers that is induced solely by adsorption of chiral molecules. In this case, about $10^{13}$ electrons per $cm^2$ are sufficient to induce magnetization reversal. The direction of the magnetization depends on the handedness of the adsorbed chiral molecules. Local magnetization switching is achieved by adsorbing a chiral self-assembled molecular monolayer on a gold-coated ferromagnetic layer with perpendicular magnetic anisotropy. These results present a simple low power magnetization mechanism when operating at ambient conditions.

## MEMS and NEMS Group
## Room 24 - Session MN+EM+NS-MoA
### Nano Optomechanical Systems/Multiscale Nanomanufacturing

**Moderators:** Robert Ilic, National Institute of Standards and Technology (NIST), Meredith Metzler, University of Pennsylvania

1:40pm **MN+EM+NS-MoA-1 GHz Integrated Acousto-Optics***, Mo Li,* University of Minnesota **INVITED**

Integrating nanoscale electromechanical transducers and nanophotonic devices potentially can enable new acousto-optic devices to reach unprecedented high frequencies and modulation efficiency. We demonstrate acousto-optic modulation of a photonic crystal nanocavity using acoustic waves with frequency up to 20 GHz, reaching the microwave K band. Both the acoustic and photonic devices are fabricated in piezoelectric aluminum nitride thin films. Excitation of acoustic waves is achieved with interdigital transducers with periods as small as 300 nm. Confining both acoustic wave and optical wave within the thickness of the membrane leads to improved acousto-optic modulation efficiency in the new devices than that obtained in the previous surface acoustic wave devices. In a photon-phonon waveguide, we further demonstrate strong Brillouin scattering of light by electromechanically excited acoustic waves. Our system demonstrates a novel scalable optomechanical platform where strong acousto-optic coupling between cavity-confined or guided photons and high frequency traveling phonons can be explored.

2:20pm **MN+EM+NS-MoA-3 Coupling Piezoelectric MEMS to Cavity Optomechanics***, Kartik Srinivasan,* NIST **INVITED**

Establishing a link between the radio frequency (RF) and optical domains is a topic of relevance to a variety of applications in communications, metrology, and photonic quantum information science. Acoustic wave devices represent an opportunity to mediate such transduction in a chip-integrated format. The approach we are pursuing uses materials that are both piezoelectric, to couple RF waves to strain fields, and photoelastic, to couple strain fields to optical waves.

One architecture that we have recently explored is based on exploiting these effects in GaAs. First, interdigitated transducers (IDTs) convert 2.4 GHz RF photons into 2.4 GHz propagating surface acoustic waves. These acoustic waves are routed through phononic crystal waveguides and are coupled to a nanobeam optomechanical cavity that supports both a highly localized 2.4 GHz breathing mechanical mode and a high quality factor 1550 nm optical mode. In contrast to non-resonant excitation of photonic structures with IDTs, here the phononic waveguide preferentially excites a localized mechanical mode, which in turn strongly interacts with the optical mode through the photoelastic effect. Finally, the optical mode can be out-coupled or excited via an optical fiber taper waveguide. Using this platform, we demonstrate preparation of the breathing mode in a coherent state at any location in phase space, and optically read out an average coherent intracavity phonon number as small as one-twentieth of a phonon. In the time-domain, we show that RF pulses are mapped to optical pulses, forming a resonant acousto-optic modulator with a sub-Volt half-wave voltage. We also observe a novel acoustic wave interference effect in which RF-driven motion is completely cancelled by optically-driven motion, enabling the demonstration of interferometric opto-acoustic modulation in which acoustic wave propagation is gated by optical pulses.

While the above platform has been shown to provide a coherent interface between the RF, optical, and acoustic domains, the overall efficiency is limited by imperfect matching across the various interfaces, e.g., IDT-to-

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[1] **Falicov Student Award Finalist**

[2] **National Student Award Finalist**

phononic crystal waveguide, etc. In the final part of my talk, I will outline efforts to improve upon the transduction efficiency of the system.

3:00pm **MN+EM+NS-MoA-5 Collective Nano-optomechanics for Sensing Applications***, **Eduardo Gil Santos**, W Hease,* Universite Paris Diderot, France*; A Lemaitre,* Centre de Nanosciences et Nanotechnologies, France*; M Labousse, C Ciuti, G Leo, I Favero,* Universite Paris Diderot, France

Optomechanical resonators have been the subject of extensive research in a variety of fields, such as sensing, communication and quantum technologies. Our recent investigations on the capabilities of optomechanical semiconductor disk resonators to operate as sensors in liquids have revealed an astonishing potential. Minimum mass detection of $14\cdot10^{-24}$ g, density changes of $2\cdot10^{-7}$ kg/m$^3$ and viscosity changes of $5\cdot10^{-9}$ Pa·s, for 1s integration time, are extrapolated from our measurements in liquids.

After landmark experiments realized on single resonators, the use of multiple optomechanical cavities is essential to further improve their sensing capabilities, as it enlarges the sensing area while keeping their individual assets. This evolution towards collective nano-optomechanics hence bears potential for a variety of sensing applications, but for quantum or topological photonics as well. Unfortunately, the collective configurations are usually impeded by the residual disorder imposed by nanofabrication techniques, which naturally detunes high optical Q resonators and precludes resonant interactions between them. Therefore, overcoming fabrication imperfections and allowing spectral alignment of resonators is essential.

Here, we develop a new simple and scalable post-fabrication method to achieve such alignment in a permanent manner. The method introduces an approach of cavity-enhanced photoelectrochemical (PEC) etching in a fluid (gas or liquid). This resonant process is highly selective and allows controlling the resonator size with sub-pm precision, well below the material's interatomic distance. Light resonantly injected into the optical mode of an optical resonator immersed in a fluid triggers an etching process, leading to a fine-tuning of the resonator's dimensions. The evolution of dimensions is monitored continuously by tracking the resonator's optical resonance with a laser. This tuning process is naturally scalable to multiple resonators. We demonstrate it using a cascaded configuration where optomechanical disk resonators, each supporting its own localized optical and mechanical mode, are unidirectionally coupled through a common optical waveguide. The technique is illustrated by finely aligning up to five resonators in liquid and two in air, opening the way of fabricating large networks of identical resonators.

As an example of application of this tuning technique, we explore the resonant optical interaction of multiple nano-optomechanical systems. We observe a first form of collective behavior involving several distant resonators, where a unidirectional flow of light frequency-locks a chain of nano-optomechanical oscillators.

3:20pm **MN+EM+NS-MoA-6 Microporous Nanophotonic Mechanical Cantilevers for Mass Sensing***, **Anandram Venkatasubramanian**, V Sauer, J Westwood-Bachman,* University of Alberta and The National Institute for Nanotechnology, Canada*; K Cui, S Roy, M Xia,* National Institute for Nanotechnology, National Research Council, Canada*; D Wishart,* University of Alberta, Canada*; W Hiebert,* University of Alberta and The National Institute for Nanotechnology, Canada

The Gas chromatography (GC) – Mass spectrometry (MS) system is the industry benchmark in chemical analysis. However the large size of the Mass spectrometry unit makes it unsuitable for portable applications. Hence a portable universal mass sensing device that can be used with portable GCs needs to be developed. In this regard, recent demonstration with nano opto-mechanical system (NOMS) devices in conjunction with a GC system have proven that these kinds of sensors have the breakthrough potential to improve the sensitivity of portable GCs. Those demonstrations using NOMS devices have shown these sensors to match the mass detection limits of nanoelectromechanical systems (NEMS) sensors and can potentially better their performance owing to their superior displacement sensitivity compared to NEMS.

In this regard, a free space interferometry system based nanophotonic sensor was developed and attached to a conventional GC. The nanophotonic sensor consists of a microring racetrack resonator (for concentration sensing) with a nanomechanical beam (for mass sensing) adjacent to it. Common method to improve the sensitivity of a nanomechanical beam is to apply surface coatings. However, the application of surface coatings can potentially affect its universal sensing characteristics. Hence an alternate way to improve the adsorption sensitivity is to increase the surface area of the nanomechanical sensor to aid in increasing the number of gas adsorption sites.

In this paper we increase the surface porosity of nanomechanical beam by stain etching. Care was taken to protect the adjacent microring resonator from stain etching as surface pores can negatively affect the performance of the ring resonator due to increased scattering. The stain etching was conducted using vanadium oxide/Hydrofluoric acid based chemistry to etch ~ 10nm pores of random morphology on the surface. Based on an estimated porosity of <15% by volume, we have noted an increase in mass adsorption of ≥ 50 - 100% when tests were conducted using different volatile organic compounds. In other words, a mass adsorption enhancement factor of 1.5 to 2 has been achieved. Due to this enhanced adsorption, the mass detection threshold has improved by an order of magnitude (~$10^{-19}$ g). To the best knowledge of the authors, this is the first time NOMS based porous nanomechanical mass sensor has been developed.

Mass Adsorption Enhancement Factor = Adsorption frequency shift for porous beam/Adsorption frequency shift for non porous beam

4:00pm **MN+EM+NS-MoA-8 Tunable Resistivity in Inkjet Printed Circuit by Plasma Reduction of Particle-free, Stabilizer-free Ink***, Y Sui, S Ghosh, C Miller, M Sankaran, **Christian Zorman**,* Case Western Reserve University

Inkjet printing offers a low-cost, rapid methodology to produce patterned metal thin films on flexible substrates. The most commonly used ink consists of colloidal suspensions of nanoparticles prepared by wet chemical reduction of metal salts. Even after concentrating the nanoparticles through solution processing, the as-printed ink usually exhibits a low conductivity due to the presence of organic molecules that help stabilize the nanoparticles from agglomeration and precipitation. High temperature (>200 C) treatment is then required after printing to remove the insulating organics and sinter the nanoparticles. The thermal step can limit printing on polymers such as PDMS, paper, and 3D printed polymers.

Here, we present a particle-free, stabilizer-free ink and a low-temperature plasma reduction process to produce electrically conductive metallic patterns on temperature-sensitive without any additional thermal step. The ink is comprised of a metal salt, a solvent, and a viscosity modifier, and is absent of any large organic molecules that cannot be evaporated after printing. The as-printed and dried metal salt is then treated with a plasma formed in a low-pressure argon environment. Even without the presence of highly reactive atomic and molecular hydrogen, this process is found to be sufficient to reduce the metal salt to highly conductive metal with resistivities approaching bulk values. More importantly, we found the resistivity of the printed structure can be tuned over a range of 2 orders of magnitude by varying the plasma power and treatment time. Thus far, we have demonstrated this general approach for silver (Ag) and tin (Sn) from silver nitrate (AgNO3) and tin (II) chloride (SnCl2), respectively. Details of the material properties as assessed by materials characterization and electrical conductivity measurements, device application to RC filter circuits, and applicability to other metals will also be discussed.

4:20pm **MN+EM+NS-MoA-9 Cold Forming of Shallow Spherical Micro Caps by Nano Imprinting***, **Asaf Asher**, E Benjamin, L Medina, S Lulinsky,* Tel Aviv University, Israel*; R Gilat,* Ariel University, Israel*; S Krylov,* Tel Aviv University, Israel

Many nonlinear systems are distinguished by bistability, which manifests itself as the coexistence of two equilibria under the same loading. Progress in the development of micro and nano structures stimulated renewed interest in the mechanics of bistable elements. Applications of these devices in the realm of micro and nanoelectromechanical systems (MEMS/NEMS) include switches, sensors, non-volatile memories, micro-pumps, micro-resonators and deformable mirrors. While curved beam-type bistable micro structures were intensively investigated both theoretically and experimentally much less attention was paid to two-dimensional bistable structures such as initially curved plates and shells (caps). One of the reasons is that lithography-based processes commonly used in MEMS/NEMS are essentially planar and are not suitable for fabrication of cap-like structures with an out-of-plane curvature. Existing approaches include gray-scale lithography or a glass blowing technique.

In this work we discuss several approaches for fabrication of shallow micro shells. One of the directions is the use of the cold forming techniques, when stamping changes a flat thin foil of ductile material into double-curvature components. While multiple variations of this process were used at the macro scale, much less works reported the implementation of this technique in MEMS. In the framework of the fabrication process used in our work, a layer of Al or Cu is deposited on top of a Si wafer. Sputtering is implemented for the creation of a thin seed layer, followed by electrodeposition used to increase the layer thickness to a desired value. Next, an opening is etched through the wafer using deep reactive ion etching (DRIE). Finally, the forming process is performed using nano-imprinting lithography tool. The tool allows very precise control of the force applied to the structure as well as the stamp temperature, displacements and rate of loading. Finite elements analysis and compact reduced order models are used for the evaluation of the desired parameters. Prior to forming, residual stress of the thin suspended membranes is estimated using a resonance method, by means of comparison of the measured natural frequencies of the device with the model predictions. We discuss suitability of different structural materials, deposition methods and stamping techniques for the formation of non-planar three-dimensional micro structures.

4:40pm **MN+EM+NS-MoA-10 Plate Mechanical Metamaterials: The Thinnest Plates You Can Pick Up by Hand***, Igor Bargatin,* University of Pennsylvania **INVITED**

Recently, my group has demonstrated a new class of ultra-lightweight plate-shaped mechanical metamaterials, which we named "plate mechanical metamaterials". Using a periodic three-dimensional patterning, we fabricated free-standing plates up to 1 cm in size out of aluminum oxide (alumina) films as thin as 25 nm. Weighing as little as 0.1 gram per square meter, they are among the thinnest and lightest freestanding solids that can be handled with bare hands. We also combined multiple ultrathin layers of alumina to create a nanoscale analog of paper-based corrugated cardboard. Unlike cardboard, these plates have the ability to “pop back” to their original shape, without damage, even after undergoing multiple sharp bends by more than 90 degrees.

Like the nanotruss -based mechanical metamaterials reported by other groups, plate mechanical metamaterials are extremely lightweight and resilient due to their nanoscale thickness and microscale cellular structure. However, in contrast to the cube-shaped metamaterials that typically form a lattice easily penetrated by the ambient air, our plates form flat continuous plates. Ultralow weight, mechanical robustness, thermal insulation, as well as chemical and thermal stability of alumina make plate metamaterials attractive for numerous applications, including structural elements in flying microrobots, high-temperature thermal insulation in energy converters, testing of nanoscale strength enhancement, new types of optical and acoustic metamaterials, as well as ultrathin MEMS/NEMS sensors and ultra-lightweight hollow MEMS/NEMS resonators.

## Electronic Materials and Photonics Division
## Room 14 - Session EM+NS-TuM

### Nanostructures and Nanometer Films for Electronic and Photonic Devices

**Moderators:** Jessica Hilton, RHK Technology, Joseph Tischler, U.S. Naval Research Laboratory

8:00am **EM+NS-TuM-1 Spin Properties in Semiconductor Colloidal Quantum Dots*, Efrat Lifshitz,*** Russell Berrie Nanotechnology Institute, Solid State Institute, Israel **INVITED**

Colloidal semiconductor quantum dots (CQDs) have been at the forefront of scientific research for more than two decades, based on their electronic and optical tunable properties. Recent years show a substantial interest in spin properties with significant importance for spin-electronic, spin-photovoltaic and spin-optical devices.

The talk includes the study of two different CQD platforms: (1) CQDs from the II-VI semiconductors and their diluted magnetic derivatives; (2) Halide perovskite CQDs. Both systems show intriguing spin properties of special scientific and technological interests.

**Spins in CdSe/CdS and $Mn^{+2}$@CdSe/CdS**: Unpaired spins generated by an absorption of a phonton (electron and hole) can dictate the magneto-optical properties of the host CQDs. Furthermore, magnetic doping by foreign ions (e.g., Mn), induces internal spin interactions between photo-generated species and the dopant spins, leading to giant magnetization. The current study developed a method to position the Mn ions selectively either at the core or at the shell, by which, controlling the electron-guest versus hole-guest exchange interaction. The materials were characterized by magneto-optical methods, including optically detected magnetic resonance, uncovered individual interactions with resident carriers, thus, revealing understanding of a control of a magnetism with a benefit for spin-based devices.

**$APbBr_3$ (A=$Cs^+$, methylamonium)*:** The perovskites are minerals that have been studied extensively in the past. They are the focus of new interest in recent years, due to their exceptional performance in photovoltaic cells. Perovskites semiconductors possess high absorption coefficients as well as long-range transport properties. Currently, they are also prepared in the form of CQDs with very interesting properties including ferroelectricity, magnetism and exciton effects. The magneto-optical measurements of excitons in $APbBr_3$ as individuals were investigated by monitoring the micro-photoluminescence spectra in the presence of an external magnetic field, while monitoring either the circular or linear polarization components. Gradual band splitting occurring upon the application of a magnetic field, deviating from a common Zeeman interaction behavior, proposes the existence of a more complex mechanism, when Rashba split is one of the plausible interpretations.

*Collaboration with M. Kovalenko and A. Rappe

9:00am **EM+NS-TuM-4 A Platform for Growth of Crystalline Thin-Film Compound Semiconductors on Oxides, Metals, and 2-D Materials*, Rehan Kapadia,*** *D Sarkar, W Wang,* University of Southern California

The electronic and photonic circuits and systems that form the backbone of the modern world are predicated on the ability to create high quality semiconductors. Yet, high-performance electronic and photonic grade semiconductors are nearly exclusively grown on lattice matched substrates. This substrate limitation arises due to the fundamental mechanisms of nucleation and growth in state-of-the-art vapor phase growth techniques, which proves to be extremely limiting and costly. Here we demonstrate a platform for growth of compound semiconductors from microscale liquid metal templates. Using these templates, we can control nucleation and growth of these compound semiconductors, enabling single crystalline devices on non-epitaxial substrates. To grow single crystalline material in the desired form-factors, from liquid metal templates on arbitrary substrates presents a significant challenge, as dewetting of the liquid films prevent control over the ultimate material geometry. Through a basic thermodynamic approach, we show that it is possible to control dewetting on nearly any material, and subsequently grow compound semiconductors on these same substrates. Using this approach, we demonstrate growth and characterization of crystalline InP, InAs, and GaP, on silicon nitride, graphene, gadolinium oxide on silicon, and metals.

Next, we show that compound semiconductors with multiple stable phases can be grown phase-pure using this approach, using tin phosphide as the example. We show that through tuning the growth conditions, we can control which stable phase of tin phosphide precipitates and grows. This control illustrates that our approach is useful for materials beyond simple III-V and II-IV compounds, which only have one stable phase. By carrying out these growths at significantly non-equilibrium conditions, we demonstrate ternary InGaP alloys, with stoichiometry control over nearly the entire In-Ga composition range. Unlike binary III-V or the Sn-P system, where the stoichiometry of the precipitating compound is nearly insensitive to the growth conditions, the ternary systems are alloys, and consequently extremely sensitive to growth conditions, making growth of uniform materials a potential challenge. We show that through control over the growth conditions, we can achieve high-quality, uniform stoichiometry ternary III-V alloys. Finally, we show that by enabling nanoscale phase segregation during growth of these ternary alloys, we can materials with extremely broadband photoluminescence curves, with FWHMs greater than 600 meV, potentially enabling a new class of broadband light sources.

9:40am **EM+NS-TuM-6 Nanometer Thick Diffused Metal Oxide Light Sensing Film Structures*, Fred Cadieu,*** Queens College of CUNY and Graduate Center of CUNY*; J Monaco,* Queens College of CUNY*; L Mourokh,* Queens College of CUNY and Graduate Center of CUNY

Approximately 10 nm thick light sensing film structures have been fabricated by sequentially sputtering various metals in oxygen, then in argon, and then in oxygen again. The layers have been deposited onto heated silicon substrates to create a diffusion region. The layered thicknesses were calibrated by x-ray reflectivity measurements. The film layers, being mostly oxides, exhibit a high lateral resistivity so that the current path is through the film thickness between a grid of contacts deposited below and on top of the film structures. For such current, a high degree of light sensitivity, and voltage polarity sensitivity, has been observed.[1] Analogous film structures have been fabricated using hafnium,[2] titanium,[2] and aluminum such that exposure to light causes large increases in currents for one voltage polarity, but little or no effect for the opposite polarity. The observed phenomenology has been shown to be consistent with a single-particle model based on the existence of interface states on the metal-oxide interfaces.[2] The details of light sensitivity and current polarity sensitivity are dependent on the deposition temperatures and thicknesses of the film layers. Hafnium based interfaces respond repeatedly to light pulses with current pulses up to several hundred microamperes, while aluminum based interfaces can only respond repeatedly with current pulses up to several tens of microamperes.

1. F.J. Cadieu, Device with Light-Responsive Layers. US Patent No. 9,040,982.

2. F.J. Cadieu and Lev Murokh, Nanometer Thick Diffused Hafnium and Titanium Oxide Light Sensing Film Structures, *World Journal of Condensed Matter Physics***7**, 36-45 (2017).

11:00am **EM+NS-TuM-10 Integration of Metallic Nanoparticles in Sensing and Memory Devices for Resistance Modulation and Enhanced Switching*, Dimitris Tsoukalas,*** National Technical University of Athens, Greece **INVITED**

In this work we present the fabrication of metallic nanoparticles (NPs) in vacuum at room temperature and their incorporation into sensor or memory two terminal devices emphasizing their influence on device resistance modulation or switching. Nanoparticles were manufactured using the gas phase condensation technique with a target of high purity. The NPs production system consists of a smaller vacuum chamber (Nanogen) which is connected via an aperture of diameter ~ 3 mm with a larger central vacuum chamber in which the sample holder is mounted. The Nanogen chamber is equipped with a DC magnetron sputtering head and in between the Nanogen chamber and the central chamber there is a pressure gradient, the pressure in the Nanogen being around $10^{-1}$ mbar while in the main chamber pressure is $10^{-4}$ mbar. The atoms produced by the magnetron sputtering because of the high pressure in the Nanogen chamber, undergo a short free path, colliding with the atoms of the inert gas (Ar) and lose part of their kinetic energy. This leads to the creation of a supersaturated vapor of the target material, which is condensed, causing the atoms to form nuclei from the material. Due to the pressure gradient prevailing, these nuclei move towards the central chamber. During this movement they interact among them to form larger NPs finally entering into the central vacuum chamber through the aperture.

Regarding the application of nanoparticle networks to sensors, our group is focusing in the use of metallic NPs in particular for chemical, bio and strain sensing applications. We first review the principle of operation of such devices that is based on the change of percolation current through the NP network when the interspace distance among NPs is modified by an external stimuli. We then discuss the potential of integrating these sensors on flexible substrates as well as the influence on their performance of a protective aluminum oxide coating deposited over the nanoparticle network.

Resistive switching memories (RRAM) based on metal oxides are emerging as a new research field and at the same time are intensively studied as one of the most promising candidates for future non-volatile memory applications. We demonstrate that a wide range of non-volatile memory properties can be affected and improved by embedding NPs into the metal oxide matrix. The concentrated electric field effect around the nanoparticles in combination with the charge trapping effect, are regarded as the driving forces for the recorded switching patterns. As a result NPs increase the on/off switching ratio and at the same time decrease the inherent variability of RRAM.

11:40am **EM+NS-TuM-12 Thin-film Metallic Glass: An Effective Diffusion Barrier for Microelectronic Packaging, CIGS Solar Cell and Thermoelectric Modules***, C Yu,* National Taiwan University of Science and Technology, Taiwan, Republic of China*; H Wu,* National Sun Yat-sen University, Taiwan, Republic of China*; **Jinn Chu**,* National Taiwan University of Science and Technology, Taiwan, Republic of China

Thin film metallic glass (TFMG) with its amorphous nature is of great interest owing to its unique properties, including high strength, large elastic limits, excellent corrosion and wear resistance. For many electronics, the atomic inter-diffusion may cause device failure or performance degradation during either fabrication or operation. Thus, the introduction of diffusion barrier layer in the device is a common approach to solve this problem. Crystalline Ni- or Ti-based layers are the most common materials for diffusion barriers. Nevertheless, grain boundaries are generally considered as atomic diffusion path, and thus crystalline metals are not able to block diffusion effectively. TFMG, possessing grain boundary-free structure, is thus thought to efficiently mitigate atomic diffusion.

In this presentation, we report the effects of thin film metallic glass as diffusion barriers on the Sn whisker mitigation in the Cu-Sn couples and the copper indium gallium selenide (CIGS) solar cells on stainless steel (SS) as well as the mid-temperature thermoelectric module. We found that TFMG effectively blocks the Cu/Sn interaction even with the thickness as thin as 25 nm. In addition, with very thin thickness, the introduction of TFMG layer is expected to yield insignificant degrees of compressive stress, which is anticipated to occur when the samples are exposed to thermal cycling. Furthermore, the detrimental iron diffusion from SS into CIGS is found to be effectively hindered by the introduction of a 70-nm-thick TFMG barrier; the cell efficiency is thus from 2.73 for bare sample to 5.25% for the one with TFMG barrier. For application in thermoelectric module, a 200 nm-thick Zr-based TFMG, acting as an effective diffusion barrier layer with low electrical contact resistivity, was deposited on a high-zT Se-doped $AgSbTe_2$ substrate. The reaction couples structured with TFMG/TE were annealed at 673 K for 8–360 hours and analyzed by electron microscopy. No observable intermetallic compounds were formed at the TFMG/TE interface, suggesting the effective inhibition of atomic diffusion.

12:00pm **EM+NS-TuM-13 Ultra-Fast Silicon Photodiodes Achieve High Efficiency via the Integration of Light-trapping Micro-/nanoholes***, **Hilal Cansizoglu**, Y Gao, K Polat, S Ghandiparsi, C Bartolo Perez, A Kaya, H Mamtaz, A Mayet,* University of California, Davis*; E Ponizovskaya Devine,* W&WSens Devices, Inc.*; T Yamada,* University of California, Santa Cruz*; A Elrefaie, S Wang,* W&WSens Devices, Inc.*; S Islam,* University of California, Davis

Surface-illuminated photodiodes (PDs) for ultra-fast data transmission are typically GaAs-based non-CMOS compatible detectors. Silicon (Si) has long been ignored for being a material of choice in ultra-fast communication links due to its poor responsivity for the wavelengths >800 nm at data rates 10 Gb/s or higher. Recent demonstration of CMOS compatible surface-illuminated Si PDs with photon-trapping micro-/nanoholes paves the way for the use of Si at 25 Gb/s or higher data transmission rate. Such PDs provided ≤30 ps full-width at half-maximum (FWHM) and above 50% quantum efficiency (QE) at 850nm, which is over 400% higher than the QE that a similar Si PD without absorption-enhancement micro-/nanoholes can provide. The micro/nanoholes create an ensemble of modes that radiate laterally by photon trapping and slow light effects, resulting in absorption enhancement in a very thin layer of Si (<2µm) which is required for high speed operations. The broadband efficiency enhancement by photon-trapping micro-/nanoholes enable Si to be considered as the PD material at longer wavelengths (>870 nm) which is below the room temperature bandgap of GaAs. Such broadband and enhanced efficiency of Si integrated with micro-/nanoholes can be useful for applications such as short wavelength division multiplexing (SWDM, 850-980 nm) for data centers, automotive laser radar systems (LIDAR, 850 or 905 nm) and high-performance computers (990-1065 nm). The CMOS-compatible fabrication of micro-/nanoholes can allow Si PDs to be monolithically integrated with CMOS/BiCMOS integrated circuits such as transimpedance amplifiers, equalizers, limiting amplifiers and other application specific integrated circuits (ASIC), which can increase the achievable data rate to more than 50 Gb/s.

## MEMS and NEMS Group
## Room 24 - Session MN+BI+EM+SS+TR-TuM

### Microelectromechanics: Relays to RF/Surfaces in Micro- and Nano- Systems

**Moderators:** Sushma Kotru, University of Alabama, Roya Maboudian, University of California at Berkeley

8:00am **MN+BI+EM+SS+TR-TuM-1 The Industrialization of MEMS through Materials Innovations***, **Chris Keimel**,* Menlo Micro **INVITED**

For the past 150 years, the mechanical relay was one of the original building blocks of electrical systems, for power electronics, controls, and even computing. With the introduction of the transistor in the middle of the 20th century, many industries were transformed with the introduction of ubiquitous, low-cost switches (solid-state) that could be manufactured by the billions with highly advanced equipment and manufacturing processes. Still today, many industries, especially power distribution and controls, are still not able to live with the tradeoffs of solid-state technologies (leakages, losses, lack of air-gap, thermal) and continue to employ large, slow, and costly mechanical relays which have evolved only slightly over the past 50+ years. The miniaturization of the mechanical relay through MEMS technology, coupled with materials innovations, will enable a new class of devices capable of connecting (wireless control) and controlling (distributed power) today's and the futures billions of automated electrical nodes.

We have developed electrostatically actuated MEMS relays capable of switching in ~3usec, sustaining more than 400V across its open contacts and controlling loads of 10s of watts to a few kilowatts. Ohmic MEMS switch with creep resistant metal alloy beams, and a highly reliable ruthenium contact has been developed based on methodical failure mode analysis taking into account material, mechanical and electrical constraints. The ohmic relays, when applied to RF applications, deliver multi throw configurations capable of <0.3dB insertion loss from DC to 3GHz combined with the ability to handle 25W of RF power.

A metal MEMS switch technology has been developed from the ground up through material, process, device, package and electronic integration innovations. The combination of fast microsecond switching speed and broadband (DC to RF) signal operation along with the ability to control amperes of current and sustain hundreds of volts across micron sized air gaps has enabled the miniaturization of the mechanical relay for broad ranging applications from wireless infrastructure to the Industrial IOT.

8:40am **MN+BI+EM+SS+TR-TuM-3 Electron-Phonon Waltz: Acoustoelectrics in MEMS***, **Dana Weinstein**,* Purdue University **INVITED**

The Acoustoelectric (AE) effect is a result of the interaction between free charge carriers and the electrical deformation potential produced by a propagating elastic wave in the piezoelectric. When an external DC electric field is applied across the semiconductor in the direction of the propagating wave, a drift velocity ($v_d$) is imparted to the free carriers. If the drift velocity is slower than (or opposite to) the acoustic wave velocity ($v_s$), the electrical deformation potential lags behind the strain wave. This phase lag not only decreases the acoustic wave velocity, but also transfers energy from the acoustic wave to the electrons, increasing the acoustic losses. When a sufficient DC field is applied to cause the drift velocity to exceed the acoustic wave velocity, the electrical deformation potential now leads the strain wave. This transfers energy from the electrons to the acoustic wave, resulting in an increased acoustic velocity and net acoustic gain [1,2,3,4].

A large body of work based on AE was established in the 1960s and 70s, resulting in a range of devices from phase shifters to correlators. With the development of new materials and new processing needs, there has been a recent resurgence of interest in this field, particularly for its amplifying and inherently non-reciprocal properties. Here, we discuss the implications of the AE effect for GHz frequency electromechanical signal processing. RF applications, linearity, and noise of the AE effect will be examined. Finally, benefits and limitations of prospective semiconductor/piezoelectric material systems will be discussed.

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9:20am **MN+BI+EM+SS+TR-TuM-5 Autonomous Oscillations of a MEMS Resonator***, **David Czaplewski,*** Center for Nanoscale Materials, Argonne National Laboratory*; C Chen, D Lopez,* Argonne National Laboratory*; D Zanette,* Centro Atomico Bariloche and Instituto Balseiro*; S Shaw,* Florida Institute of Technology

Resonant MEMS and NEMS structures are used in a wide variety of applications including mass and force sensing, time keeping, and quantum information. For all MEMS and NEMS resonators, energy is lost every cycle of oscillation to the environment (modeled as a coupled bath). If this energy is not restored by an external source, the amplitude of the resonant motion will decrease toward zero. This well-known effect is commonly referred to as “ring-down”. For linear resonators, the frequency of the resonator will remain constant and the amplitude will decreases exponentially while for non-linear resonators, the amplitude will decrease exponentially and the frequency will simultaneously decrease toward the linear response due to the amplitude-frequency (a-f) effect. However, we demonstrate a non-linear resonator that has constant frequency and an amplitude that does not decay for a given period of time (~ 0.1 s) after discontinuing the restoring energy to the system. We call this time “coherence time” because the amplitude and frequency of the oscillation does not decay when the restoring energy is removed. In essence, the resonator is autonomous during coherence time. Unfortunately or fortunately, this behavior does not violate the second law of thermodynamics. The behavior can be explained by looking at the entire system. We drive a non-linear MEMS resonator to a frequency where the primary mode couples with another internal mode. When the resonator is actively driven, the higher order mode receives energy from the primary mode. When the external energy is discontinued, this energy is restored back to the primary mode allowing the primary mode to continue to oscillate. However, once the energy stored in the higher order mode is depleted (its amplitude is near zero), the behavior of the primary mode begins to “ring-down”. During this talk, I will show characteristics of the coupled modes including operation with constant frequency and a non-decaying amplitude for a period of time with no drive.

9:40am **MN+BI+EM+SS+TR-TuM-6 Metallic Glass for MEMS Microphone Device***, **MaiPhuong Nguyen,*** WPI-Advanced Institute for Materials Research (WPI-AIMR)/ Micro System Integration Center (µSIC), Tohoku University, Japan*; J Froemel,* WPI-Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, Japan*; S Tanaka,* Graduate School of Engineering/ Micro System Integration Center (µSIC), Tohoku University, Japan

Micro Electro-Mechanical Systems (MEMS) microphones have been extensively developed and introduce into mobile phones market with high performance such as high signal to noise ratio, good sensitivity, and power consumption and good reliability in term of packages. Up to now, most studies have been focused on the improvement of sensitivity of microphone which is proportional to the compliance of the membrane. However, no significant progress has been achieved due to the limitation of material itself. Generally, single crystal and polycrystalline silicon based devices are brittle and fracture causing the interior defects during the fabrication processes. Therefore, the research of new materials to substitute polycrystalline silicon is necessary. Amorphous metals exhibit no grain boundaries, crystal defects and excellent mechanical properties such as fatigue free, large elastic limit, high strength, corrosion resistance which has been promising materials for MEMS devices such as micro-scanner, RF MEMS varactor, capacitive switch ... Metallic glasses are a kind of amorphous alloy exhibiting viscous flow at a certain temperature range so-called “supercooled liquid region”. In the supercooled liquid region, metallic glasses can be easily produced through a variety of fast-cooling methods and have excellent mechanical formability. In addition, metallic glass thin films are easily prepared on Si or $SiO_2$ substrates by sputtering technique which is compatible with MEMS processes such as photolithography, dry or wet etching and lift off processing. Therefore, characterization and fabrication of metallic glasses films deposited by sputtering for MEMS microphone will be studied.

The CoTaB films with thicknesses in the range of 100 nm to several micrometers have been successful deposited on thermal SiO2 substrates by rf-sputter technique. The amorphous structure with smooth surface and negligible magnetic property was confirmed by TEM, AFM, XRD and SQUIDS measurement, respectively. The metallic glass behavior was investigated by DSC analysis which shows the glass transition and crystalline temperature of 700 and 720.9 C, respectively. In addition, the mechanical properties such as stress, stress gradient and Young modulus have been studied by using pointer and cantilever structure. Co-based metallic glass exhibited tensile and compressive stress depending on sputter conditions, thicknesses as well as further treatment process. Additional results will be presented in detail at the conference with an emphasis on the dependence of the process conditions.

11:00am **MN+BI+EM+SS+TR-TuM-10 Role of Surfaces in Assembly of Ceria Nanostructures***, **Sudipta Seal,*** University of Central Florida **INVITED**

Cerium is a rare earth element of the lanthanide series with a fluorite lattice structure. The cerium atom can exist in either 3+ or 4+ states, and may alternate between the two in a redox reaction that is more pronounced in nanoparticles. However, the physicochemical properties of a nanocrystal assembly can be different from the properties of both the individual nanoparticles and the bulk phase. We have synthesized ceria nanoparticles in various medium and studied the self-assembly of particles to octahedral and star shaped nanostructure assembly. It was further identified that the concentration of Ce4+ in nanoceria decreases over time, further controlling the surface chemistry. We will also highlight some of the key aspects of self-assembly of $CeO_2$ into nanorods. The surface area available and the orientation of crystallographic planes in ceria nanostructures highly regulate the catalytic property at nanoscale as evident by high resolution TEM. Further we discuss the role of Madelung energy and its relation to the catalytic activity, which is important in sensing and other analyte interactions. The surface chemistry or the ratio of $Ce^{3+}/Ce^{4+}$ can be extensively modulated by the assembly process. At the end we report, the feasibility of a novel $H_2O_2$ based electrochemical sensor that directly measures the current response of multivalent ceria in presence of $H_2O_2$. The fabricated sensor showed a picomolar range limit of detection while remaining insensitive to interfering species. Peroxide sensing is very important in biologically relevant oxidative stress in cells. It was observed that a lower ratio of $Ce^{3+}$:$Ce^{4+}$ redox states elicits a greater current response towards $H_2O_2$ The detection of such electroactive analytes make it easier to detect using normal nanoparticle modified electrodes, thereby eliminating the use of organic mediators.

11:40am **MN+BI+EM+SS+TR-TuM-12 Optimization and Nano-characterization of Electrostrictive Response of Gd-doped Ceria Actuators***, **Sidney Cohen,** E Mishuk, E Makagon, E Wachtel, K Rechav, R Popovitz-Biro, I Lubomirsky,* Weizmann Institute of Science, Israel

Gd-doped ceria (GDC) recently attracted great interest due to its non-classical (non-Newnham) electrostrictive behavior. Although the material is well-known for its ionic conduction properties and use in solid-oxide fuel-cells, it also holds great promise for incorporation into MEMS devices because it is completely inert with respect to silicon compounds. The fact that GDC is lead-free is particularly appealing.

Here, we demonstrate fabrication and testing of membrane actuators formed with near 100% yield by a relatively simple, low temperature process. Preparation of these devices involves magnetron-sputtering of a thin film of GDC onto Si, and further processing using standard micromachining, resulting in free-standing membranes. Bridge and cantilever structures have been fabricated as well, to explore the possibility for diverse functional devices. The films were structurally characterized by electron microscopy and by x-ray diffraction, whereas electrical characterization was performed using impedance spectroscopy and cyclic voltammetry. These electrical tests revealed details of the conduction mechanism, role of the contacts, and charge-trapping.

Scanning probe microscopy was applied to quantitatively characterize the energetics and mechanics of the electromechanical response: Displacement of a circular membrane was measured by recording displacement of the cantilever probe under feedback as a function of frequency and applied voltage, and temporal Joule heating recorded using a scanning thermal probe. These measurements support calculations of heat-induced strain at high frequencies. These measurements showed that displacements obtained are sufficient for practical applications and provided insights on the factors controlling performance.

12:00pm **MN+BI+EM+SS+TR-TuM-13 Sustainable Thermoregeneration of Plastrons on Superhydrophobic Surfaces*, Tomer Simovich,*** Ruhr-University Bochum, Germany*; J Arnott,* The University of Melbourne, Australia*; A Rosenhahn,* Ruhr-University Bochum, Germany*; R Lamb,* Canadian Light Source, Canada

A popular and desirable function of superhydrophobic coatings is their remarkable ability to retain an entrapped layer of air, called a plastron, when submerged underwater. The drawback is that the air layer is short lived due to solvation into the surrounding liquid. Liquid gas extraction has been explored for the purpose of respiration through oxygen filtering or generation via chemical reaction. Manipulating solubility through temperature has been attempted but due to its inefficiencies has not been developed further into functioning technologies. This paper introduces a novel method of extracting gas from water to generate enough air to permanently stabilize a plastron on superhydrophobic surfaces for sustained anti-fouling, rust resistance and drag reduction abilities. This method involves locally heating the liquid surrounding a superhydrophobic coating, reducing gas solubility causing the gas to migrate to the liquid-air interface. Due to the low surface energy of superhydrophobic coatings, nucleation of supersaturated gasses occurs preferentially at the coating interface, thereby replenishing the plastron. This requires a relatively low energy input, due to the small volume of water required to be locally heated combined with the small temperature differential induced between substrate and liquid. This process may be more environmentally sustainable in comparison to competing methods. With a constant supply of equilibrated water and minimal energy input, the plastron can survive indefinitely without need for the mechanical application of additional gas.

## Nanometer-scale Science and Technology Division
## Room 19 - Session NS+EM+MI+SS-TuM

### Nanoscale Electronics and Magnetism

**Moderators:** Keith Brown, Boston University, Aubrey Hanbicki, Naval Research Laboratory

8:00am **NS+EM+MI+SS-TuM-1 Nanometrology and Nanocharacterization in Nanoelectronics*, Alain C. Diebold,*** SUNY Polytechnic Institute **INVITED**

As the so called technology node for integrated circuits moves below 10 nm, new transistor and interconnect materials as well as new device structures are moving from research into development. Pseudomorphic semiconductor films such as $Si_{1-x}Ge_x$ on Si are expected to transition to $Ge/Si_{1-x}Ge_x/Si$ or to III-V epilayers. The current lithographic processing used to pattern FinFETS is based on the Quadruple Spacer Patterning process which can result in two values of pitch walking. This greatly complicates in-line metrology. The FinFET itself will likely be replaced by nanowire transistors having multiple vertically stacked nanowire channels. Another alternative is the nano-sheet transistor. Beyond these evolutionary changes, longer term devices based on 2D materials are being investigated. These include graphene, transition metal dichalcogenides, and topologically protected materials. This talk will cover the advanced measurements being used to address the challenges associated with these new materials and structures. The talk will cover measurement methods including high resolution X-ray diffraction (XRD), XRD reciprocal space mapping, Mueller Matrix spectroscopic ellipsometry base scatterometry, and advanced electron microscopy.

9:00am **NS+EM+MI+SS-TuM-4 Measurement of Resistance Induced by a Single Potassium Atom on Chiral-Angle Known Nanotubes: Understanding the Impact of a Model Scatterer for Nanoscale Sensors*, Masahiro Ishigami,*** University of Central Florida*; R Tsuchikawa,* University of Utah*; D Heligman,* Ohio State University*; B Blue,* University of Central Florida*; Z Zhang,* Columbia University*; A Ahmadi, E Mucciolo,* University of Central Florida*; J Hone,* Columbia University

Even atomic impurities are expected to impact device properties of carbon nanotubes. Such sensitivity makes them ultimately useful for sensor technologies. Rational design for nanotube-based sensors requires precise understanding of how impurities impact transport properties of nanotubes. Such impurity-induced carrier scattering is expected to be dependent on the chirality of nanotubes and the nature of scattering potentials imposed by impurities. Yet until our recent measurements, it has been impossible to measure the impact of impurities on resistance of carbon nanotubes with known chirality.

We have developed arrays of experimental techniques to control experiments down to atomic scale to measure the scattering strength of charged impurities on semiconducting single-walled carbon nanotubes with known chirality. The resistivity of nanotubes is measured as a function of the density of adsorbed potassium atoms, enabling the determination of the resistance added by an individual potassium atom. Holes are scattered 37 times more efficiently than electrons by an adsorbed potassium atom. The determined scattering strength is used to reveal the spatial extent and depth of the scattering potential for potassium, a model Coulomb adsorbate, paving way for rational design of nanotube-based sensors. Our results are published in Phys. Rev. B [94, 045408 (2016)].

9:20am **NS+EM+MI+SS-TuM-5 Atomic Electronics for Quantum Computing*, Michelle Simmons,*** University of New South Wales, Australia **INVITED**

Extremely long electron spin coherence times have recently been demonstrated in isotopically pure Si-28 [1] making silicon one of the most promising semiconductor materials for spin based quantum information. The two level spin state of single electrons bound to shallow phosphorus donors in silicon in particular provide well defined, reproducible qubits [2] and represent a promising system for a scalable quantum computer in silicon. An important challenge in these systems is the realisation of a two-qubit gate, where we can both position donors with respect to each other for controllable exchange coupling and with respect to charge sensors for individually addressing and reading out the spin state of each donor with high fidelity.

To date we have demonstrated using scanning tunneling microscope hydrogen lithography how we can precisely position individual P donors in Si [3] aligned with nanoscale precision to local control gates [4] and can initialize, manipulate, and read-out the spin states [5,6] with high fidelity. We now demonstrate how we can achieve record single-electron readout fidelity for each of two donor based dots of 99.8%, above the surface-code fault tolerant threshold. We show how by engineering the quantum dots to contain multiple donors we can achieve spin lifetimes up to 16 times longer than single donors. Finally we show how by optimising the interdonor separation and using asymmetric confinement potentials we can create controllable exchange coupling in these devices. With the recent demonstration of ultra-low noise in these all epitaxial devices [7] these results confirm the enormous potential of atomic-scale qubits in silicon.

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11:00am **NS+EM+MI+SS-TuM-10 Electronically Abrupt Borophene/organic Lateral Heterostructures*, Xiaolong Liu*[1] [2]***, *Z Wei, I Balla, A Mannix,* Northwestern University*; N Guisinger,* Argonne National Laboratory*; E Luijten, M Hersam,* Northwestern University

Two-dimensional (2D) boron, known as borophene, has recently been experimentally realized[1,2] following theoretical predictions.[3] As an elementary 2D material, borophene is determined to be metallic like graphene, but also possesses a high degree of in-plane anisotropy like phosphorene. Thus far, all experimental studies have been performed on borophene alone, whereas borophene-based electronic applications will require precise integration of borophene with other materials. Here, we demonstrate the self-assembly of a borophene/organic lateral heterostructure[4]. Upon the deposition of perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA) on sub-monolayer borophene on Ag(111), the molecules preferentially self-assemble into monolayers on bare Ag(111), forming borophene/PTCDA lateral heterostructures spontaneously. This phenomenon is consistent with a lower adsorption energy of PTCDA molecules on borophene, as modeled via molecular dynamics simulations. The formation of the heterostructure leaves the chemical integrity of

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[1] **National Student Award Finalist**

[2] **NSTD Student Award Finalist**

borophene unperturbed as supported by in situ X-ray photoelectron spectroscopy. In addition to structural properties, atomic-scale ultra-high vacuum scanning tunneling microscopy and spectroscopy reveal strong electronic contrast between the two materials and an electronically abrupt heterojunction with a transition distance of ~1 nm (i.e., approximately the size of one PTCDA molecule). Across this transition region, the differential tunneling conductance curves change from the metallic electronic structure of borophene to the semiconducting molecular orbitals of PTCDA, suggesting the formation of an atomically abrupt 2D metal-semiconductor junction. Overall, the results of this study are likely to inform future research on borophene functionalization for nanoelectronic applications.

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11:20am **NS+EM+MI+SS-TuM-11 Mechanical Characterization of Heat Dissipation in a Current-driven Ferromagnetic Resonance System***, S Cho, M Jo, S Park, J Lee, C Yang, S Kang,* Seoul National University*; **Yun Daniel Park**,* Seoul National University, Republic of Korea

Heat dissipation in current-driven ferromagnetic resonance (FMR) system is characterized by monitoring the mechanical resonance, which shifts are governed by thermoelastic properties. Realization of a free-standing Permalloy (Py)/Pt bilayer strip, with an added mechanical degree of freedom, advantageously integrates means to separately measure mechanical resonance, by piezoresistive transduction in Pt [1], and FMR by using the spin-torque FMR (ST-FMR) measurement technique [2]. Heat generated by the precessing magnetization under an electric driving current are selectively investigated by monitoring the mechanical resonance shift, which are immune and independent to thermoelectric effects. By comparing the angular dependence to the applied magnetic field direction of the two FMR spectroscopies, ST-FMR and mechanical heat reaction, we find that Joule heat resulting from a time-dependent magnetoresistance, which in turn arises from the precessing magnetization and electrical current, cannot be overlooked in addition to the intrinsic FMR heat dissipation.

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11:40am **NS+EM+MI+SS-TuM-12 The Exciting Physics of Spin Chains Coupled to a Metallic Substrate***, **Roland Wiesendanger**,* University of Hamburg, Germany **INVITED**

A magnetic nanowire on the surface of a spin-orbit coupled s-wave superconductor is a fascinating platform, which has been proposed for observing the emergence of zero-energy Majorana bound states at the ends of the wires [1]. Majorana fermions can encode topological qubits and ultimately provide a new direction in topological quantum computation [2]. Most recently, evidences for topologically non-trivial end-states were experimentally found for self-assembled ferromagnetic Fe nanowires on superconducting Pb(110) substrates by using scanning tunneling microscopy and spectroscopy (STM/S) as well as non-contact atomic force microscopy methods [3-6]. However, self-assembled nanowires of Fe on Pb surfaces have unavoidable limitations, such as (1) intermixing of atomic species of the nanowire and the substrate during the annealing process, and (2) uncontrolled length and orientation of the nanowires.

Here, we demonstrate the fully-controlled bottom-up fabrication of artificial 1D atomic chains from individual magnetic Fe adatoms on high spin-orbit coupled non-superconducting Pt(111) and superconducting Re(0001) substrates by utilizing STM-based atom-manipulation techniques at T=350 mK. Spin-polarized STM measurements indicate the presence of non-collinear spin textures, i.e. spin spiral ground states, stabilized by interfacial Dzyaloshinskii-Moriya interactions similar to self-assembled Fe chains on Ir(001) investigated earlier [7]. The problem of intermixing is avoided by the low-temperature fabrication of the chain and an appropriate choice of the substrate, while single-atom manipulation allows the construction of chains with a given number of atoms and orientation. Tunneling spectra measured spatially resolved on the Fe-atom chain on Re(0001) reveal the evolution of the local density of states (LDOS) inside the superconducting gap as well as the development of zero-energy bound states at the ends of the chain, which are distinguishable from trivial end states by systematically increasing the number of atoms within the Fe-atom chain. The experimental results will be compared with model-type calculations supporting the interpretation of the spectroscopic signatures at the ends of the chains as Majorana bound states.

(work done together with Howon Kim and Khai Ton That).

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## Electronic Materials and Photonics Division
## Room 14 - Session EM+SS-TuA

### Surface and Interface Challenges in Semiconductor Materials and Devices

**Moderator:** Anthony Muscat, University of Arizona

2:20pm **EM+SS-TuA-1 Selective Atomic Layer Deposition of $MoSi_x$ -on Si (001) in Preference to Silicon Nitride and Silicon Oxide***, **JongYoun Choi**, C Ahles,* University of California, San Diego*; R Hung, N Kim,* Applied Materials, Inc.*; A Kummel,* University of California, San Diego

As MOSFETs size shrinks to <10 nm in a three dimensional structure (FinFET), electrical losses at the contacts must be minimized. Consequently, selective atomic layer deposition (ALD) of transition metal disilicides are of great interest due to their ability to minimize parasitic resistance and avoid lithograph onto a three dimensional structure. Selective ALD of metallic tungsten (W) via a fluorosilane elimination process have been demonstrated using $WF_6$ and $SiH_4$ or $Si_2H_6$.[1,2] This selectivity was achieved by an inherently favorable reactivity of the precursors on hydrogen-terminated Si versus OH-terminated $SiO_2$. In this W deposition process, $SiH_4$ was used as a reducing agent for W while the reactions byproducts was $SiF_4$. Here, we demonstrated that sub-stoichiometric silicide, $MoSi_x$ (x=0.4 – 1.1), can also be selectively deposited on H-terminated Si (001) in preference to SiOx and SiN using $MoF_6$ and $Si_2H_6$. X-ray photoelectron spectroscopy (XPS) was used to investigate the chemical composition of $MoSi_x$ ateach experimental step. It was observed that Si-H terminated silicon allowed single cycle nucleation of $MoSi_x$ at the substrate temperature of 100-120°C in contrast to an inherent chemical passivation (non-reactivity) on $SiO_x$ and SiN surfaces. To enable formation near stoichiometric $MoSi_x$, excess amount of $Si_2H_6$ was dosed after 5 ALD cycles to incorporate more Si into the $MoSi_x$ film while maintaining selectivity since the $SiO_x$ was unreactive to even high doses of $Si_2H_6$. This substrate-dependent selectivity was retained up to 5 - 10 ALD cycles. By applying a mixture gas of ($H_2$+$MoF_6$) instead of $MoF_6$ dosing, (as previous shown by Kalanyan et al[2]), the inherent selectivity was greatly improved and the nucleation of $MoSi_x$ was impeded up to at least 20 ALD cycles on SiN without perturbing $MoSi_x$ deposition on silicon. The growth rate of $MoSi_x$ on Si was ~0.8 Å/cycle; therefore, even 10 selective ALD cycles is sufficient for deposition of contacts. To confirm an *in-situ* selective deposition as well as the thickness of the film, $MoSi_x$ was deposited on a sample patterned with Si and SiON and the cross-section of the patterned sample was quantified using transmission electron microscopy (TEM). The surface morphology and roughness were measured using *ex-situ* atomic force microscopy (AFM) and *in-situ* scanning tunneling microscopy (STM). $MoSi_x$ on Si was conformal and atomically flat surface with root mean square (RMS) of 2.8 Å. Post-annealing in a ultra-high vacuum at 500°C for 3 mins further decreased the RMS roughness to 1.7 Å.

1. Thin Solid Films, **241**, 374 (1994)

2. Chem. Mater., **28**, 117-126 (2016)

3:00pm **EM+SS-TuA-3 Interface and Border Traps, their Passivation and the Reliability of Alumina Dielectric / Indium Gallium Arsenide Gate Stacks***, **Paul McIntyre**,* Stanford University **INVITED**

Both interface defects and border traps - charge traps in the gate oxide - influence the behavior of InGaAs metal-oxide-semiconductor (MOS) devices. This presentation will summarize the different effects of interface and border traps on the temperature- and bias-stress behavior of aluminum oxide/InGaAs MOS gate stacks, and will describe methods for passivating these defects both prior to and after gate dielectric deposition. The influence of local interface chemistry and the complex role of hydrogen as a defect passivant are highlighted.

In one set of experiments, a temperature dependent border trap response for $Al_2O_3$ gate dielectrics is investigated. This behavior is unexpected for defects that have typically been reported to charge and discharge through direct tunneling of electrons from the n-type substrate. Temperature dependent border trap frequency dispersion of the accumulation capacitance and conductance is found to be correlated with the presence of a defective interfacial layer, which can be intentionally produced either by excessive exposure to hydrating or oxidizing species during atomic layer deposition of $Al_2O_3$ or by use of a previously-reported aqueous HCl clean of the InGaAs surface prior to ALD. These results point out the sensitivity of the temperature dependence of the border trap response in metal oxide/III-V MOS gate stacks to the presence of processing-induced interface oxide layers, which alter the dynamics of carrier trapping at defects that are not located at the semiconductor interface.

We also report on the effects of pre- and post-atomic layer deposition (ALD) defect passivation with hydrogen on the trap density and reliability of $Al_2O_3$/InGaAs gate stacks. Reliability is characterized by capacitance-voltage hysteresis measurements on samples prepared using different fabrication procedures and having different initial trap densities. Despite its beneficial ability to passivate both interface and border traps, a final forming gas ($H_2$/$N_2$) anneal (FGA) step is found to induce a significant hysteresis. This is caused by hydrogen depassivation of defects in the gate stack under bias stress, supported by the observed bias stress-induced increase of interface trap density, and strong hydrogen isotope effects on the measured hysteresis. Additional strategies, beyond hydrogen annealing, for more stable interface defect passivation on InGaAs will be discussed briefly.

4:20pm **EM+SS-TuA-7 Controlling GaAs and Si Oxide Surface Energies***, **Karen L Kavanagh**,* Simon Fraser University, Canada*; N Herbots, A Brimhall, R Van Haren, Y Pershad, S Suhartono, E Landeros, R Culbertson,* Arizona State University*; R Islam,* Cactus Materials

Bonding two different semiconductors into a single integrated device can yield economic, medical, and human benefits by increasing performance. Si and GaAs bonding can increase solar cell efficiency and, if the bonding is hermetic, the lifetime of bonded sensors and optoelectronic circuits is extended by reducing percolation. Bonding occurs when the electronic properties of the two surfaces complement each other, to enhance efficient electron transfer.[1] Complementary surfaces can be identified through measurement of their total surface energy, $\gamma^T$, since this property can be modeled by Van Oss theory, to consist of three component interaction energies: molecular dipoles (Lifschitz-Van der Waals), $\gamma^{LW}$, electron donors, $\gamma^-$, and electron acceptors, $\gamma^+$. Measurements of the total and individual components of the surface energy of Si and GaAs (100) surfaces has been carried out using contact angle measurements of liquid drops with known surface energies, ranging from polar (18 MW water), apolar (α-bromo-naphthalene) to non-polar (glycerin). Accurate reproducible results are obtained using class 100 clean-room environments and analysis of multiple drops of each type of surface energy. This three liquid contact angle analysis (3LCAA) brings a much greater level of sophistication to this well-known and apparently-simple method. When carried out with semiconductor-level control of cleanliness, the contribution of each component to the total surface energy of Si (100) native and non-native oxides has been found to depend linearly on $\gamma^{LW}$. In hydrophobic oxide surfaces, $\gamma^T$ is due almost entirely to molecular interactions, $\gamma^{LW}$, to within a few % error. Thus, the highly-passivated, thermally-grown $SiO_2$ surface with few defects or impurities, has a surface energy of 35.7 ± 3 mJ/m$^2$ that is entirely explained by $\gamma^{LW}$. However, $\gamma^T$ can be raised to 57.3 ± 2 mJ/m$^{2.}$ by generating defects, and unsaturated or dangling bonds that interact with electron acceptors and or donors. This situation applies to heavily-etched, oxide surfaces, or chemically-oxidized surfaces. The contributions from $\gamma^-$and $\gamma^+$, raises the total surface energy $\gamma^T$ up to 40% above that of $\gamma^{LW}$, which is found to remain nearly constant. Similar experiments with GaAs (100) surfaces as a function of surface preparation find that the Si-doped GaAs native oxide to be hydrophobic with a $\gamma^T$of 35 ± 3 mJ/m$^2$, with $\gamma^{LW}$contributing 98 ± 2%, thus close to the entirety of $\gamma^T$. This indicates a well-reacted native oxide. [1] *Herbots N. et al. US Patent 9,018,077 (2015); 9,589,801 (2017).*

4:40pm **EM+SS-TuA-8 *In Situ* $Si_3N_4$ Surface Layer on GaN-on-Si Heterostructure for High Power Operation***, **Chien-Fong Lo**, O Laboutin, X Gao, C Kao, H Marchand, W Johnson, R Pelzel,* IQE

Gallium nitride based devices have been delivering their promise of high power and high frequency operation as a capable replacement for silicon based devices, applications, owing to highly desirable III-nitride physical properties [1] . However, device performance is limited by excessive Schottky gate leakage, which results in high gate subthreshold leakage and leakage instability. These in turn cause high off-state drain leakage, a degradation of power efficiency, and ultimately device reliability problems.

Schottky leakage is caused by an excessive trap states density at the interface between the Schottky gate and the nitride semiconductor, resulting in excess negative charges on the barrier surface and/or in the barrier layer that induce current collapse in off-state operation. Dielectric capping of the III-nitride structure is one method to suppress the gate leakage in both forward and reverse bias, thereby mitigating current collapse and further improving the 3-terminal breakdown. Passivation with silicon nitride has been reported to reduce the current collapse and provide a relatively low state density at the $SiN_x$/III-N interface [2] and is widely used. However, in many instances, the $SiN_x$ passivation is done *ex-situ* from the GaN epi system which results in an oxide layer at the nitride/$SiN_x$ interface, which in turn reduces the efficacy of the passivation. Therefore, it is desirable to perform the $SiN_x$ deposition *in-situ* so that the semiconductor/$SiN_x$ interface is oxide-free.

*In-situ*, MOCVD $SiN_x$ films have been grown on 100–200 mm Si substrates and characterized with RBS, AFM, XRD/XRR, and *C-V* profiling. Stoichiometric silicon nitride films with good surface morphology and material properties have been achieved. Metal-insulator-semiconductor HEMT (MISHEMT) devices with *in-situ* $SiN_x$ capping layer were fabricated and compared with conventional GaN-capped HEMTs. Devices with *in-situ* passivation exhibit three orders of magnitude lower gate leakage current and improved 3-terminal breakdown (200V improvement at 10 µA/mm, see Fig. 1). Hall–Van der Pauw measurements performed on both GaN- and $SiN_x$-capped samples indicate that using *in-situ* $SiN_x$ results in a significant increase in channel carrier density, which is consistent with $SiN_x$ providing a reduced trap state density at the Schottky/semiconductor interface [3]. Additional electrical data including pulsed *I-V* will be presented to validate the improvements in switching performance. All of the nitride-based materials and $SiN_x$ passivation layers have been grown using a commercial MOCVD reactor ensuring cost-effective implementation for commercial power-switching applications.

5:00pm **EM+SS-TuA-9 In-Vacuo Studies of Surface Structure and Surface Chemistry During Plasma-Assisted Atomic Layer Epitaxial Growth of InN Thin Films on GaN Substrates***, **Samantha Rosenberg**,* ASEE (residing at NRL)*; D Pennachio,* University California Santa Barbara*; V Anderson,* ASEE (residing at NRL)*; N Nepal,* U.S. Naval Research Laboratory*; C Wagenbach,* Boston University*; A Kozen,* ASEE (residing at NRL)*; Z Robinson,* SUNY Brockport*; J Logan, S Choi,* University California Santa Barbara*; J Hite,* US Naval Research Laboratory*; K Ludwig,* Boston University*; C Palmstrøm,* University California Santa Barbara*; C Eddy, Jr.,* U.S. Naval Research Laboratory

III-N semiconductors are well suited for applications in several important technological areas, including high current, normally-off power switches.[1-3] Such devices require heterostructures not readily achievable by conventional growth methods. While atomic layer deposition (ALD) is a versatile technique and has gained wide use, it does not offer the required level of crystallinity and purity for high-performance III-N semiconductor devices. Therefore, we have developed a technique adapted from ALD, called plasma-assisted atomic layer epitaxy (ALEp).[2]

Here we employ i*n-situ* and *in-vacuo* surface studies of GaN substrate preparation and InN ALEp growth to advance fundamental understanding of the ALEp process. We conduct *in-situ* grazing incidence small angle x-ray scattering (GISAXS) experiments at the Cornell High Energy Synchrotron Source, utilizing morphological evolution monitoring to investigate the growth interface during sample preparation at several different temperatures and film deposition at growth temperature. GISAXS information is complemented with *in-vacuo* x-ray photoelectron spectroscopy and reflection high-energy electron diffraction studies conducted at the Palmstrøm Lab at UCSB, where we consider traditional molecular beam gallium flash-off and atomic hydrogen etching as ways to produce the most suitable GaN surface for our ALEp-based approach.

1. N. Nepal, et al., Appl. Phys. Lett. 103, 082110 (2013)

2. C. R. Eddy, Jr, et al., J. Vac. Sci. Technol. A 31(5), 058501 (2013).

3. R. S. Pengelly, et al., IEEE Trans. Microwave Theory Tech. 60, 1764 (2012).

5:20pm **EM+SS-TuA-10 Aqueous Ammonium Sulfide Treatments on SiGe Surfaces***, **Stacy Heslop**, L Peckler, A Muscat,* University of Arizona

Employing germanium (Ge) and/or silicon germanium (SiGe) as the active material in transistors has the potential to generate electronics that are faster and consume less power. The narrower band gaps and higher hole mobilities compared to silicon make these materials ideal candidates for the next generation of microelectronics, but their integration into current manufacturing is difficult due to the rapid oxidation of germanium. These oxides are unstable, electrically defective, and form a poor interface with the underlying substrate hindering their electrical performance. The native $GeO_2$ is water soluble and unable to protect the surface during liquid phase processing. To combat this, the oxidation is prevented by depositing a thin sulfide layer to chemically passivate the surface. Ammonium sulfide is a common passivation reagent due to the size and valency of the sulfur atom and its ease of integration into current industrial processes. X-ray photoelectron spectroscopy (XPS) was used to study the effect of varying concentrations of aqueous ammonium sulfide on SiGe. No sulfide layer was detected for surfaces treated with aqueous ammonium sulfide and instead the surface reoxidized in solution. Hydrofluoric and hydrochloric acids were added to the ammonium sulfide solution to remove or prevent the formation of these oxides in solution. Samples treated with ammonium sulfide with added acid showed a sulfide layer. Increasing the concentration of HF and HCl increased the sulfur coverage but also increased the oxide coverage, suggesting the deposition of oxidized sulfur species.

Metal-insulator-semiconductor capacitors (MISCAPs) were fabricated for three different surface treatments. Capacitance –voltage and conductance data was used to quantify the density of interface defects ($D_{it}$). Samples treated with ammonium sulfide with added acid showed the highest sulfur coverage and had fewer interface defects ($1.4 \times 10^{12}$ cm$^{-2}$ eV$^{-1}$) compared to samples treated with aqueous ammonium sulfide or samples with no sulfur treatment.

6:00pm **EM+SS-TuA-12 The Structural Stability and Phase Transition of $MoTe_2$ Activated by Thermal Annealing***, **Hui Zhu**, Q Wang, C Zhang, R Addou, K Cho, M Kim, R Wallace,* University of Texas at Dallas

Among group-VIB transitional-metal dichalcogenides (TMDs), semiconducting molybdenum ditelluride (2H-$MoTe_2$) with a similar bandgap to Si (~1.1 eV for monolayer and 1.0 eV for bulk state), is a promising candidate for electronic and photovoltaic applications.[1] Additionally, $MoTe_2$ possesses phase transition behavior, for example, the well-known phase transition between its semiconducting 2H structure and its semimetallic, distorted octahedral 1T' structure due to their small formation energy difference (~0.03 eV).[2] The thermally induced structural stability of $MoTe_2$ needs careful evaluation for nano-electronic device applications compared to the other TMDs due to a small electronegativity difference (~0.3) between Mo and Te, which may weaken the Mo-Te bonding strength. In this work, using scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS), and scanning transmission electron microscopy (STEM), we investigated the thermal structural stability of $MoTe_2$ heated under high vacuum conditions and discovered an interesting decomposition or phase transition process from 2H-$MoTe_2$ (initial) to 2H-$MoTe_2$ surface decomposition with random Te atomic vacancies (200 °C and 300 °C) to semi-periodic, “wagon wheel” patterns of 60° inversion domain boundaries ($MoTe_{1.5}$ at boundaries, 400 °C) to one dimensional, metallic $Mo_6Te_6$ nanowires (NWs, 450 °C).[3] Particularly, the $Mo_6Te_6$ nanowires registered along the <11-20> 2H-$MoTe_2$ crystallographic directions with lengths in the micrometer range. The metallic NWs can act as an efficient hole injection layer on top of 2H-$MoTe_2$ due to the favorable band-alignment. Furthermore, an atomically sharp $MoTe_2$/$Mo_6Te_6$ interface and van der Waals gap with the 2H layers are preserved. The work highlights an alternative pathway for forming new transition metal chalcogenide phases and will enable future exploration of their intrinsic transportation properties.

This research was supported in part by the **SWAN** Center, a SRC center sponsored by the Nanoelectronics Research Initiative and NIST, and the Center for Low Energy Systems Technology, one of the six SRC STARnet Centers, sponsored by MARCO and DARPA.

**Reference**

(1) Keum, D. H.; et. al. Bandgap Opening in Few-Layered Monoclinic $MoTe_2$. *Nat. Phys.***2015**, *11*, 482–486.

(2) Cho, S.; et. al. Phase Patterning for Ohmic Homojunction Contact in $MoTe_2$. *Science.***2015**, *349*, 625–628.

(3) Zhu, H.; et. al. New $Mo_6Te_6$ Sub-Nanometer-Diameter Nanowire Phase from 2H-$MoTe_2$. *Adv. Mater.***2017**, 1606264.

## Nanometer-scale Science and Technology Division
## Room 19 - Session NS+EM+MN+PS+SS-TuA

## Nano-Photonics, Plasmonics and Mechanics

**Moderators:** Joshua Ballard, Zyvex Labs, Christian Zorman, Case Western Reserve University

2:20pm **NS+EM+MN+PS+SS-TuA-1 Nonlinear Interactions of Coupled MEMS Cantilevers*, Christopher Wallin,*** National Institute of Standards and Technology, Center for Nanoscale Science and Technology*; R De Alba, D Westly,* NIST/CNST*; S Grutzik,* Sandia National Laboratories*; A Zehnder, R Rand,* Cornell University*; V Aksyuk,* NIST/CNST*; S Krylov,* Tel Aviv University, Israel*; B Ilic,* NIST/CNST

Micro- and nano-electromechanical systems (M/NEMS) offer tremendous opportunities for technological advancement in mechanical resonator applications including mass, force and energy sensing, microwave amplification, optomechanics, and energy harvesting. These M/NEMS resonators have many favorable qualities including high mechanical quality factors and compatibility with integrated circuit architectures. More specifically, nonlinear, coupled M/NEMS resonating cantilever arrays have been shown to possess complex system dynamics such as intrinsically localized modes, wave propagation, and sensitivity to defects. The collective behavior of these nonlinear interacting cantilever arrays is remarkably sensitive to the slightest perturbation which makes them an excellent candidate for ultra-sensitive sensors. Moreover, custom device responses can be achieved by tuning the electrostatic fringing field coupling, altering the mechanical coupling via the device's overhang, or by introducing precisely engineered structural imperfections into the arrays. With our work, we have found that the cantilever arrays exhibit distinct propagation bands, abrupt transitions between standing wave patterns, and synchronization.

Various device geometries including interdigitated arrays, opposing element arrays, and di-element arrays were constructed using both silicon and silicon nitride as device layers. The arrays generally consisted of 100 cantilevers or more which limited boundary effects in the devices. Gold electrodes were patterned on top of the cantilevers for parametric electrical actuation and for fringing field electrostatic coupling between adjacent cantilevers. Mechanical coupling in the arrays was achieved through the large overhangs produced during the device release. The amplitude envelope of the out of plane motion of the cantilevers was captured using a CMOS camera using a frame rate of 30 $s^{-1}$. The devices were driven electrically and using a piezoelectric transducer under ambient and vacuum conditions. Large, nonlinear vibrational amplitudes were observed in the arrays along with hysteresis. The cantilever arrays exhibited unique standing wave patterns which were sensitive to defects and external loading. Since the dynamics of M/NEMS coupled cantilevers are highly sensitive to local changes in their environment, we envision the practical implementation of coupled arrays for ultra-sensitive chemical, biological, and force sensors in the future.

2:40pm **NS+EM+MN+PS+SS-TuA-2 Silicon Carbonitride Nanoresonator Arrays for Proteomic Analysis***, W Zheng,* University of Alberta, Canada*; R Du,* University of Alberta and The National Institute for Nanotechnology*; Y Cao,* University of Alberta and The National Institute for Nanotechnology, Canada*; M Mohammad, S Dew,* University of Alberta, Canada*; M McDermott,* University of Alberta and The National Institute for Nanotechnology***; Stephane Evoy,*** University of Alberta, Canada

Analysis of biological molecules is vital in many fundamental problems of molecular biology. ELISA is a widely employed array-based technique for the parallel analysis of biological analystes. This technique however requires fluorescent tagging, which may disrupt the biochemical properties being investigated. Other platforms such as quartz crystal microbalance (QCM) and surface plasmon resonance sensors (SPR) offer alternatives for the analysis of molecular mixtures. However, these platforms are not readily scalable towards large arrays. Resonant mechanical sensors operate by monitoring shifts of resonance frequencies associated to the binding. Such approach enables the frequency modulation of the output, improving the stability/noise-immunity of the reading. In addition, the adsorption sensitivity per unit area of resonators scales favourably as their dimensions are reduced, offering a compelling path for the development large arrays with exquisite mass-sensitivities.

Suspended silicon resonators as narrow as 45 nm were initially reported by Carr, Evoy et al.[1] The brittle properties of this material however limited the yield of these structures to less than 25 %, precluding their use in large arrays. We have recently reinvented the overall approach employed in NEMS fabrication. This new approach combines surface and bulk machining techniques for the release of the device, as opposed to the widely-accepted sacrificial layer approach. We are now routinely fabricating ultra-large arrays of SiCN nanostring resonators as narrow as 8 nm and a yield approaching 100%. These are the narrowest devices produced by any machining method. Each device offers a detection threshold as small as 200 Da. These arrays have successfully been employed for the detection and analysis of protein mixtures. Diazonium modification was developed onto the SiCN surfaces and validated by X-ray photoelectron spectroscopy. Similarly modified nanostrings were then covalently functionalized with anti-rabbit IgG as molecular probe. Specific enumeration of rabbit IgG was successfully performed through observation of downshifts of resonant frequencies. The specificity of this enumeration was confirmed through proper negative control experiments. Helium ion microscopy further verified the successful functionalization of nanostrings.

[1] D. W. Carr, S. Evoy, L. Sekaric, H. G. Craighead, J. M. Parpia, App. Phys. Lett. 75, 920 (1999).

3:00pm **NS+EM+MN+PS+SS-TuA-3 Cavity Optomechanical Coupling in Chip-Scale Plasmonic and Photonic Transducers for Nanoscale Measurements and Optical Signal Control*, Vladimir A. Aksyuk,*** *S An,* NIST Center for Nanoscale Science and Technology*; B Dennis,* Rutgers University and NIST CNST*; T Michels, B Roxworthy, J Zou,* NIST Center for Nanoscale Science and Technology **INVITED**

Devices controlling light via mechanical motion are ubiquitous, from a simple camera's zoom lens to arrays of moving mirrors correcting for atmospheric distortions in telescopes and digitally projecting movies on the cinema screens. The same optomechanical coupling provides one of the best known techniques for measuring mechanical motion, covering length scales form atomic force microscopy to kilometer scale LIGO interferometers to the red shift measurements over billions of light years. We study optomechanical coupling in micro and nanoscale systems that combine electromechanics with photonics and plasmonics, and apply such chip based optomechanical transducers to solve nanoscale measurement problems. In one example, integrated cavity-optomechanical sensing breaks the common trade-off between sensitivity and bandwidth in atomic force microscopy, allowing extremely low noise motion readout of very fast, nanoscale/picogram mechanical probes. Reducing the probe size not only increases the transduction bandwidth, but also reduces drag and therefore the fundamental thermodynamic force noise when operating in air. Even though the cantilever crossection is much smaller than the optical wavelength, the near-filed coupled high quality factor photonic cavity makes our motion readout exquisitely sensitive. As a second example, I will discuss nanomechanical plasmonic systems, where extreme confinement of the gap plasmon optical modes leads to some of the largest optomechanical coupling coefficients ever observed. I will present electro-mechanical gap plasmon phase modulators and nanomechanically tunable deep subwavelength gap plasmon resonators with potential applications for motion metrology, novel nanoscale sensing and signal transduction and arbitrary wavefront control via nanoelectromechanically tunable optical metasurfaces.

4:20pm **NS+EM+MN+PS+SS-TuA-7 An Active Plasmomechanical System for Optical Modulation and Mechanical Lasing*, Brian Roxworthy,*** *V Aksyuk,* NIST

Plasmonic structures can couple electromagnetic radiation into volumes much smaller than the limits imposed by diffraction. This strong confinement of light transforms these static metallic nanostructures into sensitive bio-chemical sensors, near-field probes for imaging, nanoscale light sources, and effective optical tweezers [1-4]. Advancing the plasmonics paradigm to include active devices, whose resonant properties can be dynamically tuned *via* various electrical, mechanical, or thermal inputs, has great potential to advance nanoscale optical sensing and transduction and for building functional metamaterial devices [5,6].

We present a tunable plasmomechanical system that couples the localized gap plasmon (LGP) resonances of individual subwavelength structures to mechanical, electrical, and thermal modes. By engineering extremely strong optomechanical coupling of the LGPs, we achieve broad tuning of the localized resonances at megahertz frequencies using small voltages < 5 V, producing ≈ 40 % amplitude in the far field and > π phase shift of the re-radiated light. We furthermore show selective, sub-diffraction optical transduction of nanomechanical motion with < 10 fm $Hz^{-1/2}$ sensitivity. Coupling of LGPs to thermal modes results in strong thermomechanical backaction capable of driving regenerative mechanical oscillations of cantilever devices – mechanical lasing – using an isolated, subwavelength plasmonic element. Our platform opens the door to smart metamaterials having programmed responses across physical domains, tunable metasurfaces and optical components, and studying optically-powered nonlinear nanomechanics.

[1] J. Anker *et al.*, Nat. Mater. 7, 442–453 (2008).

[2] D. K. Gramotnev and S. I. Bozhevolnyi, Nat. Photon., 83–91 (2010)

[3] Y-J. Lu *et al.,* Science 337, 450–453 (2012)

[4] B. J. Roxworthy *et al.,* Nano Lett. 12, 794–801 (2012)

[5] N. Zheludev and E. Plum, Nat. Nanotech. 11, 16–22 (2016).

[6] B. J. Roxworthy and V. A. Aksyuk, Nat. Commun. 7, 13746 (2016).

4:40pm **NS+EM+MN+PS+SS-TuA-8 Plasmon-enhanced Photo-catalysis Using Collapsible Nano-fingers***, **Yunxiang Wang**, B Song, W Wu, S Cronin,* University of Southern California

**1. Introduction**

Photocatalytic decomposition plays an important role in the treatment of pollutants. It utilizes light radiation to decompose contaminants into non-toxic substances. While $TiO_2$ is one of the most widely used photocatalysts, visible light can hardly be used to drive $TiO_2$ due to the short wavelength cutoff of $TiO_2$. Plasmon-enhanced photo-catalysis can extend the wavelength range due to higher order effects. However, previously reported work has limited efficiency, because the hot spots were not optimized and the $TiO_2$ located outside the hottest part of the hotspots. Here, we invented a technology to fabricate collapsible nano-fingers to achieve large-area high density optimized hotspots with $TiO_2$ film located at the hottest part of the hotspots. We demonstrated highest photo-catalysis efficiency that we are aware of.

**2. Device fabrication**

First, pillar arrays were patterned on the top two layers using UV-curable nanoimprint lithography (NIL) and reactive ion etch (RIE), as shown in Fig. 1(a) (b) (c). Au film was deposited on the sample followed by lift-off process to form gold nanoparticle arrays with diameter of 50 nm and pitch of 200 nm on the bottom layer, as shown in Fig. 1(d) (e). After nano-fingers were fabricated using RIE, 2 nm TiO2 film was deposited on the sample using atomic layer deposition (ALD), as shown in Fig. 1(f) (g). After the arrays were exposed to ethanol solutions and air-dried, the fingers closed together in groups of two or four. The scanning electron microscopic (SEM) image of the collapsed nano-fingers is shown in Fig. 2.

**3. Results and Discussion**

The photocatalytic activities were tested using methyl orange (MO) photodegradation as the model reaction. The decay in absorbance of the solution was monitored by Varian Cary 50 UV–Vis spectrophotometer after 8 h exposure to green laser (532 nm, 3 W) irradiation. MO solution and sample were added into a standard quartz cuvette sealed with a sealing film.

The absorption spectra taken before and after irradiating are used to quantify the photocatalytic decomposition rate, as shown in Fig. 3. As a control experiment, we firstly performed experiment under same illumination condition with a silicon wafer coated with 2nm $TiO_2$ film, no MO photodecomposition was observed even after 12 h irradiation. For the monomers, the absorption of the MO solution is observed to drop by 4.9% after 8 h illumination. However, with collapsed sample, a 30% reduction in the MO absorbance is observed. This over 6-fold enhancement demonstrates a stronger plasmonic enhancement after nano-fingers being collapsed, which means this novel structure is a great platform to study plasmonic enhancement.

5:40pm **NS+EM+MN+PS+SS-TuA-11 Ultra-High Resolution Photonics-based Thermometry***, **Nikolai Klimov**, T Herman, K Douglass, M Chojnacky, Z Ahmed,* National Institute of Standards and Technology

Temperature measurements play a crucial role in various aspects of modern technology ranging from medicine and manufacturing process control, to environmental and oil-and-gas industry. Among various temperature measurement solutions, resistance-based thermometry is a time-tested method of disseminating temperature standards [1]. Although industrial resistance thermometers can routinely measure temperatures with uncertainties of 10 mK, their performance is sensitive to multiple environmental variables such as mechanical shock, thermal stress and humidity. Drift of sensor resistance over time necessitates expensive, time-consuming recalibrations using ultra-sensitive reference thermometers. These fundamental limitations of resistance thermometry, as well as the desire to reduce sensor ownership cost have ignited a substantial interest in the development of alternative temperature measurement solutions such as photonics-based temperature sensors. A wide variety of innovative photonic sensors have been proposed recently including functionalized dyes [2], hydrogels [3], fiber optics-based sensors [4], and silicon micro- and nanophotonic devices [5,6]. These innovative temperature sensors have the potential to leverage advances in frequency metrology to provide cost-effective measurement solutions. Here we present the results of our efforts in developing novel on-chip integrated silicon photonic temperature sensors with nanoscale footprint and ultra-high resolution as an alternative solution to legacy-based resistance thermometers. These sensors are Fabry-Perrot cavity type silicon photonic devices that are based on photonic crystal nanobeam cavity (PhCC), whose high-Q resonant frequency mode is highly sensitive to even ultra-small temperature variations. In this talk we describe nanofabrication, fiber coupling and packaging of these thermometers, as well as their performance. We will present a direct comparison of our photonic thermometers to Standard Platinum Resistance Thermometers, the best in class resistance temperature sensors used to disseminate the International Temperature Scale of 1990. The preliminary results indicate that our PhCC nanothermometers are capable of detecting changes of temperature as small as 10 µK and can achieve measurement capabilities that are on-par or even better than the state-of-the-art resistance thermometry.

[1] Strouse, NIST Spec. Publ. 250, 81 (2008).

[2] Donner et al., Nano Lett. 12, 2107 (2012).

[3] Ahmed, J. Adv. Res. 6, 105 (2015).

[4] Kersey et al., IEEE Photonics Technol. Lett. 4, 1183 (1992).

[5] Kim et al., Opt. Express 18, 22215 (2010).

[6] Klimov et al., Proc. SPIE 9486, 948609 (2015).

6:00pm **NS+EM+MN+PS+SS-TuA-12 Size-Controlled Synthesis of Gold Nanostars and their Excellent SERS and Fluorescence Quenching Properties***, **Waqqar Ahmed**, H Khan, M Khalid,* COMSATS Institute of Information Technology Islamabad, Pakistan

Noble metal nanoparticles have attracted great attention recently owing to their fascinating optical properties. They work as nanoscopic antennas by amplifying the incident and scattered electromagnetic beam. The incident electromagnetic radiation can excite the surface plasmons of nanoparticles, leading to the confinement of electromagnetic energy around the nanoparticles. This makes the metallic nanoparticles an excellent candidate for the surface enhanced Raman scattering (SERS) applications. Anisotorpic nanoparticles such as nanostars are much superior for SERS applications over their spherical counterparts owing to the special surface morphology.

We have developed a facile method for the synthesis of gold nanostars with tunable sizes ranging from 50nm to about 1µm. To the best of our knowledge, this is the widest size range reported for gold nanostars. More importantly, we have observed that these nanostars are excellent for SERS based detection owing to their large enhancement factors and efficient fluorescence quenching properties. Fluorescence is known to interfere with and overshadow the SERS signal, thus affecting the trace detection capabilities of SERS. Therefore, usually off resonance excitation lasers must be used for SERS studies of fluorophores, which limits the universal applicability of the SERS technique. We believe that non-compact surfactant coating of nanostars in our case give the target fluorophores access to nanostar's surface, thus enabling the quenching of fluorescence through Förster resonance energy transfer (FRET). The absence of fluorescence background markedly enhances the appearance of Raman peaks. We were able to achieve a limit of detection of 10pM using an excitation laser source in resonance with the electronic excitation of the target fluoropore. This makes gold nanostars universal substrates for SERS based trace detection.

## 2D Materials Focus Topic
## Room 15 - Session 2D+EM+SS+TF-WeM
### 2D Materials Growth and Fabrication

**Moderator:** Aleksandra Radenovic, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

8:00am **2D+EM+SS+TF-WeM-1 Chemical Bath Deposition of Phase Selective MoS$_2$ on Templated Surfaces**, ***Jenny Hedlund***, *A Walker,* University of Texas at Dallas

Transition metal dichalcogenides (TMDs) have a wide range of physical properties, and consequently have applications in nanoelectronics and biosensors. While TMD materials have been well studied, a simple method for two-dimensional large area thin film deposition of these materials has yet to be achieved. Chemical bath deposition (CBD) is a robust method by which to grow uniform thin films, and offers many advantages over other techniques including low deposition temperatures (≤ 50°C), synthetic flexibility, and it is inexpensive. In this work, CBD is used to deposit large-area ultra-thin molybdenum disulfide (MoS$_2$), a group VI TMD, and the resulting deposits are investigated by scanning electron microscopy (SEM), x-ray photoelectron spectroscopy (XPS), Raman spectroscopy and time-of-flight secondary ion mass spectrometry (TOF SIMS). These TMDs are most commonly found to possess trigonal prismatic crystalline structure (2H phase) and therefore are semiconductors. Although less widely studied, TMDs can also possess octahedral crystallinity to form the 1T phase. The 1T phase exhibits different properties to the 2H phase, and has applications in sensing, metal contacts and catalysis. By using substrates that mimic the TMD crystalline structure for deposition we have shown that MoS$_2$ can be deposited with large-area crystallites observed. SEM images of deposition performed on highly oriented pyrolytic graphite show large area flakes, ~100 µm in diameter. Smooth thin films were also deposited on sapphire, and functionalized self-assembled monolayers (SAMs). XPS results show that Mo 3d and S 2s peaks are present in the expected positions and ratios. We further demonstrate that the deposited MoS$_2$ phase is likely determined by the surface chemistry of the substrate. Using Raman spectroscopy measurements, the thickness and phase of the film are elucidated. CBD of MoS$_2$ was further characterized using TOF SIMS to elucidate the reaction mechanisms as well as the stability of the deposited film.

8:20am **2D+EM+SS+TF-WeM-2 Atomic Layer and Metalorganic Chemical Vapor Deposition of MoS$_2$ and WS$_2$ from bis(tert-butylimido)-bis(dialkylamido) Compounds**, ***Berc Kalanyan***, *J Maslar, W Kimes, B Sperling,* NIST*; R Kanjolia,* EMD Performance Materials

Layered 2D transition-metal dichalcogenides (TMDs) are finding use in nanoelectronic and optoelectronic applications due to their thickness-dependent optical and electrical properties. Scalable fabrication of TMD-based devices requires vapor-phase deposition routes that can produce continuous and uniform films with sub-nanometer thickness control. Atomic layer deposition (ALD) is a desirable route for the synthesis of 2D TMDs and heterostructures due to digital thickness control achieved by sequential self-limiting surface chemistry. However, since ALD conditions are only met at relatively low deposition temperatures, most ALD films are amorphous. Some consider this a useful feature of ALD, since film growth rate and structural development can be decoupled by separating the deposition and crystallization steps. In contrast, metalorganic chemical vapor deposition (MOCVD) enables direct growth of crystalline films, but requires careful process control and precursor selection to achieve the required level of thickness control. The tradeoffs between direct CVD growth and post-sufurization and annealing of amorphous/metallic films is the focus of this work.

In this paper, we present a comparison of process characteristics and film properties, including growth rate, thickness, morphology, composition, and crystallinity, as a function of two deposition routes: ALD and MOCVD. We deposited thin films using $(N^tBu)_2(NMe_2)_2M$ and 1-propanethiol, where M={Mo,W}, at wafer temperatures of 200°C to 400°C for ALD and 400°C to 900°C for pulsed MOCVD on SiO$_2$/Si substrates. Precursor saturation conditions were evaluated using in situ infrared flow measurements and ex situ X-ray photoelectron spectroscopy. As-deposited and sulfur-annealed films were further evaluated using X-ray diffraction, optical spectroscopies, and microscopy. As-grown ALD films were amorphous and included a mixture of a sulfide and a conductive phase, likely a nitride. Below 300°C, deposition was limited to a thin surface oxide. Higher temperatures resulted in higher growth rates, which also introduced a weak CVD component to the growth. Deposition rates were <1.0 Å/cycle at 350°C. As-deposited films were successfully annealed to 2H-MoS$_2$ under a sulfur atmosphere, which also removed residual nitrogen. As-grown MOCVD films were polycrystalline 2H-MoS$_2$ at 600°C. Pulsed injections of precursor enabled Å-level control over aggregate film thickness. For both processes, wafer-scale growth and uniformity in a perpendicular flow reactor were demonstrated on 50 mm substrates. We will also present process characteristics for the analogous WS$_2$ route and discuss initial data from MoS$_2$/WS$_2$ nanolaminates.

8:40am **2D+EM+SS+TF-WeM-3 Epitaxial Growth of Atomically Thin Transition Metal Dichalcogenides and their Electronic Structures**, ***Sung-Kwan Mo,*** Lawrence Berkeley National Laboratory **INVITED**

Transition metal dichalcogenides (TMDCs) is a versatile material platform with a variety of electrical, optical, and topological properties that can be controlled through thickness, strain, field, and other perturbations. In this talk, I will first discuss the growth of atomically-thin TMDC films, such as MoSe$_2$, WSe$_2$, WTe$_2$, NbSe$_2$, and TaSe$_2$, with a layer-by-layer thickness control, using molecular beam epitaxy. Then, I will present how we investigate the electronic structures of these films using angle-resolved photoemission spectroscopy and scanning tunneling microscopy.

9:20am **2D+EM+SS+TF-WeM-5 Terminations and Treatments of Silicon Carbide Surfaces to Promote Epitaxial Hexagonal Boron Nitride Deposition by Chemical Beam Epitaxy**, ***Daniel Pennachio,*** *N Wilson, A McFadden, T Brown-Heft,* University of California at Santa Barbara*; K Daniels, R Myers-Ward, D Gaskill, C Eddy, Jr.,* U.S. Naval Research Laboratory*; C Palmstrøm,* University of California at Santa Barbara

This work examines the epitaxial deposition of single-crystal hexagonal boron nitride (h-BN) on silicon carbide substrates through the use of surface treatments which promote suitable nucleation and growth. Silicon carbide, 6H-SiC(0001), was chosen as a candidate substrate due to its market availability, high crystalline quality, temperature stability, and potential coincident lattice match to h-BN. Boron nitride was deposited in ultra-high vacuum (UHV) environments by chemical beam epitaxy (CBE) on SiC substrates through thermal decomposition of borazine at high temperatures. Different SiC surface reconstructions reached through exposure to elemental silicon and subsequent *in-vacuo* annealing were examined for their effect on h-BN nucleation and epitaxial arrangement. Along with reconstructions produced through UHV annealing, CVD-grown epitaxial graphene on 4H-SiC was also utilized as a growth surface. Growth past full single atomic layer coverage of sp$^2$-bonded material (either h-BN deposited layers or graphene substrates) proved difficult with the accessible temperature range and precursor flux. Various surface treatment approaches were investigated to promote additional layer growth.

Deposited h-BN films on the SiC reconstructed surfaces were found to be near-stoichiometric and of single- to few-atomic layer thickness, as determined by *in-situ* x-ray photoelectron spectroscopy (XPS) B1s:N1s peak area ratios and substrate peak attenuation. Progression of *in-situ* reflection high-energy electron diffraction (RHEED) during h-BN deposition provides evidence of a difference in film nucleation between the Si-rich (3x3) and the C-rich SiC surface reconstructions: while the (3x3) reconstruction quickly transitioned to a (1x1) reconstruction upon precursor dosing, the C-rich reconstruction persisted despite thicker depositions. XPS of the C-rich surface showed a higher binding energy shoulder of the C1s peak, indicative of sp$^2$-hybridized bonding in a graphene-like buffer layer at the surface. Triangular nuclei seen by scanning electron microscopy after deposition on the C-rich SiC surface suggests epitaxial arrangement to this buffer layer. *In-situ* scanning probe microscopy and *ex-situ* transmission electron microscopy were performed to acquire additional information on film morphology. The influence of different surface treatments for increasing the thickness of h-BN growth will be presented.

9:40am **2D+EM+SS+TF-WeM-6 Photo-Chemical Modification of Monolayer Transition Metal Dichalcogenides**, ***Tariq Afaneh,*** *P Sahoo, H Gutierrez,* University of South Florida

Fabrication of in-plane 2D heterostructures is a crucial step to advance in the development of a truly 2D optoelectronics. Different approaches have been attempted, including in situ sequential growth of two different materials and post-growth modification of the chemical composition in a 2D monolayer. In this work, we studied a post-growth technique that exploits the radiation-matter interaction under a controlled atmosphere. Using a homemade sealed mini-chamber with a quartz optical viewport, a laser beam (532 nm) was focused onto the sample, consisting on MoSe$_2$ or WSe$_2$, while keeping a reactive sulfur-rich atmosphere within the chamber. The spatially localized photo-chemical conversion was in situ monitored by mapping the temporal evolution of the Raman active modes. The process can be tuned thereby choosing appropriate laser power, exposure time, and reactive gas environment. The complete or partial conversion was further confirmed by collecting the photoluminescence spectra at the desired exposed sites. The time-dependent intensities of the Raman peaks were fitted to exponentially decaying functions. Depending on the reaction parameters, two different processes with distinct time constants can be identified. The following mechanisms for the photo-conversion are proposed: (i) creation of Se vacancies in the TMD materials due to the energy absorbed from the laser radiation, (ii) cracking of sulfur containing molecules from the gas environment and subsequent incorporation of the sulfur atoms into the Se vacancy sites. The optimization of this process will allow to develop techniques based on photo-induced chemical reactions for local doping, alloying and the fabrication of in-plane TMD heterostructure.

11:00am **2D+EM+SS+TF-WeM-10 Bottom-up synthesis of Graphene Nanomembranes with Tunable Porosity*, Christof Neumann,*** Friedrich Schiller University Jena, Germany*; M Füser,* Goethe University Frankfurt, Germany*; M Mohn,* Ulm University, Germany*; D Kaiser,* Friedrich Schiller University Jena, Germany*; A Gölzhäuser,* Bielefeld University, Germany*; U Kaiser,* Ulm University, Germany*; A Terfort,* Goethe University Frankfurt, Germany*; A Turchanin,* Friedrich Schiller University Jena, Germany

The potential of atomically thin materials like graphene or carbon nanomembranes (CNMs) [1] for separation or ultrafiltration technologies is based on their negligible thicknesses enabling the ballistic transport of atoms and molecules through the nanomembranes. For such implementations, large scale production of perforated nanomembranes with well-defined sizes of nanopores has to be established. Here we present a scalable method to produce atomically thin graphene nanomembranes with tunable porosity using aromatic self-assembled monolayers (SAMs) as molecular precursors. We employ N-containing 4-(1H-pyrrol-1-yl)thiophenol, 4-(2,5-dimethyl-1H-pyrrol-1-yl)thiophenol and 4-(pyrimidin-2-yl)phenylthiol SAMs on polycrystalline copper foils to convert them into CNMs via low energy electron irradiation induced crosslinking and then to pyrolyze CNMs into nanoporous graphene sheets in vacuum. We characterize the formed supported and suspended graphene nanosheets by different complementary spectroscopy and microscopy techniques including X-ray photoelectron (XPS) and Raman spectroscopy, atomic force (AFM), helium ion (HIM) and high-resolution transmission electron microscopy (HRTEM) as well as by electric transport measurements. We demonstrate that the pore size and the graphene crystallinity can be adjusted by the production parameters and discuss the mechanisms.

[1] A. Turchanin and A. Gölzhäuser, Carbon Nanomembranes, *Adv. Mater.* 28 (2016) 5075

11:20am **2D+EM+SS+TF-WeM-11 Cu Single Crystal Substrates for Growth of CVD Graphene*, Tyler Mowll,*** University at Albany, SUNY*; Z Robinson,* SUNY Brockport*; C Ventrice, Jr.,* SUNY Polytechnic Institute

To provide a systematic study of the CVD graphene growth process, a study of the growth of graphene on single crystal Cu substrates, with terminations along the (100), (110), and (111) planes, was performed. Synthesis was performed in an ultra-high vacuum (UHV) chamber using a modified setup to allow growth at pressures as high as 1 Torr. Ethylene was used as the precursor gas. To control Cu sublimation at the elevated growth temperatures, an Ar overpressure was used. This arrangement allowed for the preparation of clean Cu surfaces by sputtering and annealing the Cu crystals in UHV, followed by graphene growth at low pressure, and in-situ analysis with low energy electron diffraction. It was found that surface termination plays a strong role in the rotational alignment of the nucleating graphene grains and the decomposition rate of the ethylene. It was observed that single-domain epitaxy is possible on Cu(111) when the ethylene pressure is 5 mTorr or less. However, growth on both Cu(100) and Cu(110) result in a minimum of two domains. In addition, ex-situ EELS is currently being performed on well-ordered epitaxial graphene films grown on Cu(111) and Cu(100) to determine the effect of the graphene-Cu interaction on the electronic properties of the graphene.

11:40am **2D+EM+SS+TF-WeM-12 Paper and Circuits, only Atoms Thick*, Jiwoong Park,*** University of Chicago **INVITED**

2D layered materials are like paper: they can be colored, stitched, stacked, and folded to form integrated devices with atomic thickness. In this talk, I will discuss how different 2D materials can be grown with distinct electrical and optical properties (coloring), how they can be connected laterally to form pattered circuits (stitching), and how their properties can be controlled by the interlayer rotation (twisting). We will then discuss how these atomically thin papers and circuits can be folded to generate active 3D systems.

## Electronic Materials and Photonics Division
## Room 14 - Session EM-WeM

### Charge Transport in Disordered Materials

**Moderator:** Michelle Paquette, University of Missouri-Kansas City

8:00am **EM-WeM-1 Electrons and Phonons in Amorphous Semiconductors*, David Drabold,*** *K Prasai,* Ohio University*; P Biswas,* University of Southern MIssissippi **INVITED**

The coupling between lattice vibrations and electrons is one of the central concepts of condensed matter physics. The subject has been deeply studied for crystalline materials, but far less so for amorphous and glassy materials, which are among the most important for applications. In this talk, we explore the electron-lattice coupling using current tools of first-principles computer simulation. We choose three materials to illustrate the phenomena: amorphous silicon, amorphous selenium, and amorphous gallium nitride. In each case, we show that there is a strong correlation between the localization of electron states and the magnitude of thermally-induced fluctuations in energy eigenvalues obtained from density-functional theory (i.e. Kohn-Sham eigenvalues). We provide a heuristic theory to explain these observations. The case of amorphous GaN, a topologically disordered partly ionic insulator, is distinctive compared to the covalent amorphous systems. We close by showing how the optical gap of an amorphous semiconductor can be computationally engineered with the judicious use of Hellmann-Feynman forces (associated with a few defect states) using molecular dynamics simulations. These forces can be used to close or open an optical gap, and identify a structure with a prescribed gap. We use the approach with plane-wave density functional methods to identify the conducting state of a conducting bridge memory material: Ag-doped $GeSe_3$.

K. Prasai, P. Biswas and D. A. Drabold, *Electrons and Phonons in Amorphous Semiconductors*, Semicon. Sci. Tech. **31** 073002 (2016).

8:40am **EM-WeM-3 Percolation Resistivity in Nanostructured Transparent Conductor Networks Consisting of Curvy Nanowires*, Junying Li,*** *C Ying, J Hicks, A Ural,* University of Florida

Transparent, conductive electrodes have many applications in electronic and photonic devices such as touch screens, solar cells, LEDs, and photodetectors. Metal nanowire networks are promising candidates for these applications as a replacement for indium tin oxide, which has problems such as high cost, scarcity, and brittleness. The conduction in metal nanowire networks is governed by percolation theory.

In most computational work, nanowires in these networks have been modeled as straight “sticks”. However, in real experiments, individual nanowires are not perfectly straight, but exhibit some degree of curviness. In this work, we perform systematic Monte Carlo simulations to study the effect of nanowire curviness on the scaling of percolation resistivity in nanowire networks. We generate the curved nanowires using 3rd-order Bézier curves. These curves are endowed with a curviness angle property that specifies how far away the two intermediate control points of the Bézier curve may lie, in the tangential sense, from a straight path connecting the two ends of the curve. The curviness angle is varied to obtain networks of differing values of curl ratio, which is defined as the ratio between the curved length of a nanowire and the straight distance between its two ends.

We find that, for random networks, the resistivity of the network increases with increasing nanowire curviness and the resistivity exhibits an inverse power law dependence on the curl ratio. We also find that the value of the extracted inverse power law critical exponent is not universal, but depends on other nanowire and device parameters. As a result, we also study the effect of nanowire density, nanowire length, device length, device width, and nanowire alignment angle on the scaling of network resistivity with nanowire curl ratio.

Curviness results in two competing effects on the percolation resistivity. First, curviness decreases the effective length of the nanowire between its two ends, which increases the resistivity. Second, it increases the effective width of the nanowire, which decreases the resistivity. For networks with aligned nanowires, we find that increasing the curviness decreases the resistivity, indicating that the second effect starts to dominate. By simulating networks with varying values of alignment angles, we study the crossover from the first to the second regime.

These results show how the degree of curviness of individual nanowires contributes to the macroscopic resistivity of the network. They also show that computational studies are an essential tool for providing insight into the percolation transport in transparent, conductive nanowire networks.

9:00am **EM-WeM-4 Surface Chemical Control of Charge Transport and Infrared Plasmonic Response in Nanocrystal Thin Films***, **Dmitriy Boyuk**, W Hu, M Filler,* Georgia Institute of Technology

Infrared plasmonic nanocrystal thin films are promising materials for harvesting thermal radiation, but their use requires an ability to simultaneously control nanocrystal carrier density and interfacial charge transport. Here, we combine *in situ* infrared spectroscopy and nanoscale four-point probe measurements to show the intimate interplay between nanocrystal surface chemistry, the localized surface plasmon resonance (LSPR), and thin film resistivity. Indium tin oxide (ITO) nanocrystals synthesized via colloidal methods exhibit LSPRs tunable in the mid-infrared (from 0.2 to 0.6 eV) and serve as model infrared plasmonic materials with which to study these effects. Removal of surface hydroxyl groups, via reaction with metal alkyl species (e.g., trimethylaluminum), and formation of a monolayer of oxygen-metal surface bonds (e.g., Al-O) reduces the number of nanocrystal surface traps. The corresponding increase in carrier density is evidenced by a clear blue shift and increase in intensity of the LSPR. This monolayer surface treatment decreases nanocrystal film resistivity by two orders of magnitude (to $1 \times 10^{-2}$ ohm-cm). We further demonstrate that conformal coatings (e.g., of $Al_2O_3$ or ZnO) permit control of nanocrystal thin film resistivity without modifying LSPR energy, a capability that allows us to independently engineer light absorption and device properties. We also find that these plasmonic nanocrystal films exhibit a photoconductivity in response to mid-infrared light illumination.

9:20am **EM-WeM-5 Study of Cation Exchange and Transport in Crystalline Solids Through Density Functional Theory Calculations***, **Daniel Dumett Torres**,* University of Illinois at Urbana-Champaign

Ion transport is closely tied to chemical transformations of crystalline ionic solids such as impurity doping and ion exchange. In order to introduce heteroatoms and other impurities into a crystal it is necessary to displace ions, create vacancies, and fill vacancies many times to achieve a significant degree of transformation. Thus ionic mobility plays a deterministic role both as to how fast a transformation occurs and the achievable extent of doping/exchange in a given system. For example exchange of $Cd^{2+}$ for $Cu^{+}$ in CdSe nanocrystals occurs rapidly and full conversion is ultimately reached. However replacing $Cd^{2+}$ for $Hg^{2+}$ does not reach completion and proceeds more slowly. A full explanation for how these two processes differ must address the mobility difference between $Hg^{2+}$ and $Cu^{+}$ through the $Se^{2-}$ sublattice.

As a separate example: fast ion conduction relies on there being extensive ion transport in a solid. Such transport could be facilitated by cooperative effects, low ($<k_bT$) activation energy barriers against ion migration, or a combination of these and other factors. An understanding for how ionic mobilities differ and how they might be manipulated or enhanced will guide the design of materials such as nanoscale semiconductors for applications in optoelectronics, solid state battery electrolytes, and thermoelectrics. Specifically, control over superionic phase transitions can make new materials available for applications in solid state electrolytes by permitting new superionic conductors to be realized at working conditions as opposed to at elevated temperatures.

The approach is to employ density functional theory (DFT) electronic structure calculations for the elucidation of ion conduction trends in $Li_xCu_{2-x}Se$. The $Li_xCu_{2-x}Se$ alloys vary in their fraction of $Li^{+}$ or $Cu^{+}$ cations both of which are mobile and thus apt for a study into tuning ion mobility. Total energies from DFT calculations for a large set of $Li_xCu_{2-x}Se$ structures permit the identification of factors that promote or inhibit ion mobility. By varying both the cation locations and cell parameters the energetic penalties associated with pushing cations from their relaxed positions into interstitial sites can be obtained. Coupled with a exploration of the $Li_xCu_{2-x}Se$ compositional range, the DFT energies reveal the best alloys for cation transport that have the lowest energetic penalties and smallest activation barriers. Complementary calculations in which the simulation cell volume is increased or decreased study the effects of tensile and compressive strain respectively; the calculated energies inform how strain and pressure can be used to control ion conduction.

9:40am **EM-WeM-6 Probing Charge Transport in Amorphous Hydrogenated Boron Carbide***, **Gyanendra Bhattarai**, S Dhungana, R Thapa, T Nguyen, A Caruso, M Paquette,* University of Missouri-Kansas City

Amorphous hydrogenated boron carbide is a complex disordered semi-insulating material being studied for neutron detection applications owing to its high thermal neutron absorption cross-section and high resistivity. Optimizing its charge transport properties, including charge carrier mobility, lifetime, and mobility-lifetime product, will be essential to successful detector implementation. Tuning these properties requires a clear understanding of the disorder in this solid, as well as charge injection and hopping via localized states, and how these phenomena lead to difficulties in experimental design as well as analysis of charge transport measurements. This contribution will present an overview of the challenges and nontrivialities in establishing electrical contacts and determining charge transport properties introduced by the disorder in the material, and our approaches to measurement and analysis.

11:00am **EM-WeM-10 On the Abnormality in Mobility of ZnO Thin Film Transistors Based on Sol-Gel Deposited Channel Layers***, **Vahid Mirkhani**, K Yapabandara, S Wang, M Khanal, S Uprety,* Auburn University*; M Sk,* Qatar University, Qatar*; A Ahyi, M Hamilton, M Park,* Auburn University

Extensive research has been conducted on zinc oxide (ZnO) thin film transistors (TFTs) for the last couple of decades. Solution processes such as sol-gel are popular fabrication methods among researchers due to their simplicity and economical aspects. We have observed an abnormality in transconductance and mobility curve of the TFT with a channel layer prepared through sol gel spin coating process. Transconductance and mobility curves, determined from transfer characteristics, exhibit two peaks, instead of an expected single peak. We have rationalized the phenomenon by pondering the ZnO-ZnO interfaces. During the ZnO thin film deposition process, the spin coating and calcination steps are repeated multiple times in order to achieve a desirable layer thickness. When a layer is deposited, prior to the second spin coating step, the vacancies on the layer surface (comprised of grain boundaries of different grains) act as active sites, adsorbing molecules from the ambient. The adsorption of gasses such as oxygen and water molecules on ZnO structure surfaces has been studied for several decades; although the detailed kinetics and chemical reactions are debatable. Moisture and oxygen may be chemisorbed on the surface by receiving an electron and form a trapped negative ion on the surface, forming a depletion region at the surface of the layer. Oxygen may capture an electron and react with oxygen vacancies ($V_O$ and $V_O^{+}$), in order to form chemisorbed ions such as $O^{-}$, $O^{2-}$ or $O_2^{-}$, whereas $H_2O$ may form $OH^{-}$ on the surface. Potential barriers created at the interlayer interfaces are wider and higher than the regular barriers created at the grain boundaries in the bulk. The interlayer interface depletion layers formed by negative ions will not be affected by the annealing process due to their stability at room temperature. Thus, the initial ZnO-ambient interface (prior to the next layer-deposition process) evolves into the ZnO-ZnO interlayer interface. The significance of the depletion layers at the ZnO-ZnO interfaces becomes evident when the carriers are not able to drift across these interfaces at gate voltages smaller than a critical voltage ($V_C$). As the gate voltage increases, the width of the depletion regions decrease and carriers are able to tunnel through the barriers with ease and utilize all the deposited layers as a single channel and hence, an increase in the transconductance and mobility and later, a second peak. It is proposed that the first peak is related to the formation of the channel in the top layer and the second peak is assigned to all the deposited layers acting as a single-layer-channel.

11:20am **EM-WeM-11 Electrical Characterization and Localized Density of States Extraction of Thin-Film Transistors Based on Sol-Gel Derived ZnO Channel Layers with Different Annealing Temperatures***, **Shiqiang Wang**, R Cheng, M Hamilton, V Mirkhani, K Yapabandara, S Uprety, A Ahyi, M Park,* Auburn University*; M Sk,* Qatar University, Qatar

We report on the fabrication and electrical characterization of bottom gate thin-film transistors (TFTs) based on sol-gel derived ZnO channel layer. The effect of annealing of ZnO active channel layers on electrical characteristics of the ZnO TFTs was systematically investigated. Photoluminescence (PL) spectra indicate that the crystal quality of the ZnO improves with increasing annealing temperature. Both the device turn-on voltage ($V_{on}$) and threshold voltage ($V_T$) shift to a positive voltage with increasing annealing temperature. As annealing temperature is increased, both the subthreshold slope ($SS$) and the interfacial defect density ($D_{it}$) decrease. The field effect mobility ($\mu_{FET}$) increases with annealing temperature, peaking at 800 °C and decreases upon further temperature increase. Besides that, the temperature dependent field effect measurement (from

296 K to 330 K) was used to gain an insight on the annealing temperature effect on sol-gel derived ZnO TFTs electrical characteristics. The conduction processes in these TFTs are thermally activated and the drain current, especially in subthreshold regime, obeys Arrhenius equation. Thermal activation energy and a corresponding prefactor parameter were extracted from temperature dependent field effect measurement. The Meyer-Neldel (MN) rule widely observed in the intrinsic material property study is also obeyed by the relation between thermal activation energy and the prefactor parameter. By combing the MN rule and applying the self-consistent procedure, the localized sub-gap density of states ( DOSs) of different temperature annealed sol-gel derived ZnO TFTs were successfully extracted. The DOSs for subthreshold regime decrease from $10^{19}$ $eV^{-1}cm^{-3}$ level to $10^{17}$ $eV^{-1}cm^{-3}$ level with increasing annealing temperature from 600 ℃ to 800 ℃ and no substantial change was observed with further temperature increase to 900 ℃. The results show that DOSs decrease with annealing temperature increase in general, but annealing at a very high temperature may not be beneficial to reducing DOSs. It was found that the TFTs with ZnO layers annealed at 800 °C for one hour shows the best electrical performance with the highest field effect mobility and lowest localized DOSs.

11:40am **EM-WeM-12 Real-space Characterizations of Photo-generated Carriers in P3HT-based Nanostructures using Kelvin Probe Force Microscopy***, **Eunah Kim**, S Kwon,* Ewha Womans University, Republic of Korea*; D Kim,* Ewha Womans University, Republic of Korea, Republic of Korea*; H Park,* Korea Advanced Nano Fab Center, Republic of Korea*; J Kim,* Incheon National University, Republic of Korea*; D Kim,* Ewha Womans University, Republic of Korea

Organic-inorganic hybrid nanostructures have been proposed to improve the performance of organic photovoltaic devices. In this work, we investigated creation and transport behaviors of photo-generated carriers in P3HT-based hybrid nanostructures, such as P3HT-coated Si-nanopillar (NP) arrays and P3HT layers with embedded upconversion nanorods (UCNs). Optical resonance strongly concentrated incident light in the Si NPs, significantly increasing the number of photo-carriers near the NPs. The UCNs converted near-infrared (NIR) light to visible light . We studied spatial distribution of the surface photovoltage (SPV) in the P3HT/Si-NP and P3HT/UCN samples using Kevin probe force microscopy. The magnitude and sign of SPV are determined by the number of the photo-carriers and band profiles near the sample surface [1-3]. Large SPV values appeared in the P3HT layers near the Si NPs under illumination of visible light and near the UCNs under illumination of NIR light in the P3HT/Si-NP and P3HT/UCN samples, respectively [3,4]. This suggested that the concentrated light in the NPs and photon upconversion in the UCNs increased the local density of photo-carriers. Our work shows that the scanning probe microscopy technique can visualize the creation and transport behaviors of photo-generated carriers in nanostructures.

1. E. Kim et al., *Curr. Appl. Phys.***16**, 141 (2016).

2. M. Gwon et al., *Sci. Rep.***5**, 16727 (2015).

3. E. Kim et al., *Sci. Rep.***6**, 29472 (2016).

4. Y. Jang, E. Kim et al., *J. Phys. Chem. Lett.* **8**, 364 (2017).

12:00pm **EM-WeM-13 Electrically Detected Magnetic Resonance Study of the Relationship Between Silicon Nitride Stoichiometries and Defect Structure and Energy Levels***, **Ryan Waskiewicz,*** Pennsylvania State University*; M Mutch,* Micron Technology*; P Lenahan,* Pennsylvania State University*; S King,* Intel Corporation

Leakage currents in dielectric thin films utilized in present day integrated circuitry are important reliability concerns. Among the most important dielectric materials are amorphous hydrogenated silicon nitrides (a-SiN:H). These relatively high dielectric constant materials are utilized in many applications such as a passivating layer, an etch stop layer, a diffusion barrier to water, and a gate dielectric. Electron paramagnetic resonance (EPR) studies of a-SiN:H films have identified the K center (a silicon dangling bond back-bonded to three nitrogen atoms) as the single dominating paramagnetic defect in stoichiometric films. Previous studies of spin dependent trap assisted tunneling (SDTAT) detected via electrically detected magnetic resonance (EDMR) provide us with energy levels for these K center defects. [1] However, the effects of varying N/Si stoichiometry on defect levels and defect chemistry have not been studied with EDMR. We have initiated such an EDMR study of SDTAT in a-SiN:H dielectric samples of several stoichiometries.

In our SDTAT/EDMR measurements, a slowly varying magnetic field and an oscillating rf or microwave frequency magnetic field are applied to the thin film samples. As in conventional EPR, energy is absorbed by paramagnetic sites when the resonance condition is met. In the simplest cases, this condition may be expressed by hv=guB, where *h* is Planck's constant, g is an orientation dependent parameter often close to 2, u is the Bohr magneton, and B is the magnetic field. In EDMR, the EPR is detected through a change in current, in our case due to SDTAT.

The devices in our study include 3 nm a-SiN:H stoichiometric samples, and 25 nm a-SiN:H samples with three N/Si ratios of 1, 1.35, and 1.5. The overall device structures under observation consist of Ti/a-SiN:H/p-Si capacitors. A comparison of EDMR measurements taken at high field and frequency (X-band frequency ~ 9.75GHz, 3500G) and low field and frequency (frequency ~ 85-350MHz, 30-125G) provide us with information about defect structure. These comparisons allow us to extract information about the g matrix as well as hyperfine interactions. (The g and hyperfine details provide information about defect structure.) A comparison of EDMR measurements under various biasing conditions allow us to approximately determine the energy levels of the defects involved. This energy level and defect structure information should lead to a better understanding of transport in these technologically important materials.

[1] M.J. Mutch, P.M. Lenahan, and S.W. King, *Appl. Phys. Lett.* **109**(6), 062403 (2016).

## Sustainability Focus Topic
## Room 5 & 6 - Session SU+AS+EM+MS-WeM

## Piezoelectrics, Thermoelectrics, and Superconductors

**Moderators:** George Nolas, University of South Florida, Kimberly Cook-Chennault, Rutgers University

8:20am **SU+AS+EM+MS-WeM-2 Investigation into Novel p-type Thermoelectric Materials***, **Dean Hobbis**, K Wei, G Nolas,* University of South Florida

Novel thermoelectric materials are in high demand due to the ability to directly convert waste heat into electrical power, a process that has limitless applications both privately and commercially. Currently n-type thermoelectric materials have been more vastly studied than p-type and have been optimized to higher Figures of Merit (ZT). A thermoelectric module requires both n-type and p-type materials, therefore the efficiency of the module is characterized by the combination of ZT values. This means the optimization of p-type thermoelectric materials is extremely important to the commercial viability of thermoelectric technology. Furthermore, the particular synthesis method is also of importance for applications in industry. In skutterudites, for example, methods of fractional filling are typically used to improve thermoelectric efficiency by promoting phonon scattering to reduce thermal conductivity in the material, but most of the elements used as filler are electron donors. Nevertheless, Br is an electron acceptor when used as a filling atom [1]. In quaternary chalcogenides, thermal conductivity can be intrinsically low due to the crystal structure so methods to improve electrical transport is often employed through alloying and substitution on different atomic sites. Certain antimonides also possess intrinsically low thermal conductivity. Furthermore, differing processing conditions can influence the transport properties significantly, resulting in different ZT values. In this talk we present our latest work on these material systems, including new data that shows substantial improvement In ZT with composition and processing conditions.

[1] Nolas et al. *Mat. Res. Soc. Symp.* 626, **2001**, Z10.1.1

8:40am **SU+AS+EM+MS-WeM-3 Thermoelectrics for Sustainable Energy Harvesting***, **Mary Anne White,*** Dalhousie University, Canada **INVITED**

Thermoelectrics can convert heat to power. The key to this process is the combined electrical (high electrical conductivity and Seebeck coefficient) and thermal (low thermal conductivity) properties. Although thermoelectrics have been used commercially for more than 50 years, new materials with higher efficiency could make their use more widespread. A large fraction of energy consumed is actually wasted as heat, so efficient conversion of this waste heat to useable power would be a great advantage to humanity. After a general introduction to thermoelectrics, this presentation will focus on improvement of thermoelectrics via sustainable approaches, including consideration of sustainability of the elements, and recent work focusing on elements with high availability.

9:20am **SU+AS+EM+MS-WeM-5 Toward a Greener World: The (Re)search for Lead-Free Piezoelectrics**, ***Xiaoli Tan***, Iowa State University **INVITED**

Piezoelectricity refers to the linear coupling, in the direct effect, between mechanical stress and electric displacement, and in the converse effect, between mechanical strain and applied electric field. The proportionality constants are the piezoelectric coefficients which are equivalent between the direct and the converse effects. For the past six decades ceramics based on $Pb(Zr_{1-x}Ti_x)O_3$ (PZT) perovskite oxides have been the workhorse of piezoelectric technology due to their excellent properties, ease of processing, and low cost. The high piezoelectric performance of PZT is primarily resulted from the intrinsic lattice distortion and the ferroelectric domain switching. However, environmental concerns with lead have stimulated worldwide intensive efforts in the search for lead-free piezoelectric ceramics.

The research efforts on lead-free piezoelectric ceramics have been largely concentrated on three solid solution families: $BaTiO_3$-based, $(K_{0.5}Na_{0.5})NbO_3$-based, and $(Bi_{1/2}Na_{1/2})TiO_3$-based compositions. $BaTiO_3$-based ceramics exhibit excellent piezoelectric coefficients, but their applications are limited by their low Curie points (~100 °C). $(K_{0.5}Na_{0.5})NbO_3$-based compositions possess high piezoelectric coefficients and relatively high Curie points (> 200 °C), but have stringent requirements on the processing conditions. $(Bi_{1/2}Na_{1/2})TiO_3$-based polycrystalline ceramics develop giant electrostrains (up to 0.70%), but usually require a very high electric field.

In this presentation, an overview of the recent development in the search and research on lead-free piezoelectric ceramics will be given. Their chemical compositions, structure evolutions, and mechanisms for property optimization will be discussed. In addition, two specific investigations will be presented. The first one is on the microstructural response to poling electric fields in the $(Bi_{1/2}Na_{1/2})TiO_3$–$BaTiO_3$ solid solution. With the *in situ* transmission electron microscopy technique, it is directly observed that poling fields can either destroy or create morphotropic phase boundaries and the associated strong piezoelectric property. The second investigation is on the development of a giant electrostrain of 0.70% at 50 kV/cm at room temperature in $\{[Bi_{1/2}(Na_{0.84}K_{0.16})_{1/2}]_{0.96}Sr_{0.04}\}(Ti_{0.975}Nb_{0.025})O_3$. This polycrystalline ceramic with randomly oriented grains is even better than some single crystals in terms of some electromechanical properties. *In situ* transmission electron microscopy examination indicates that the giant electrostrain is originated from the reversible phase transitions under applied electric fields.

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11:20am **SU+AS+EM+MS-WeM-11 Thermal Annealing Effects on the Thermoelectric Properties of Si/Si+Sb Thin Films**, ***Satilmis Budak***, *Z Xiao, M Curley, M Howard, B Rodgers, M Alim,* Alabama A&M University

Thermoelectric devices were prepared from multi-nanolayered Si/Si+Sbthin films using DC/RF magnetron sputtering system. Thermoelectric devices were annealed at different temperatures to form quantum (nano) structures in the multilayer thin films to increase the Seebeck coefficients and electrical conductivity and decrease thermal conductivity. The prepared devices were characterized using Seebeck coefficient measurement; four probe van der Pauw measurement resistivity and the laser thermal conductivity systems. The surface morphology of the fabricated thermoelectric films is characterized using Scanning Electron Microscope (SEM+EDS).

**Acknowledgement**

Research was sponsored by NSF with grant numbers NSF-HBCU-RISE-1546965, DOD with grant numbers W911 NF-08-1-0425, and W911NF-12-1-0063, U.S. Department of Energy National Nuclear Security Administration (DOE-NNSA) with grant numbers DE-NA0001896 and DE-NA0002687.

11:40am **SU+AS+EM+MS-WeM-12 Critical Current by Design**, ***George Crabtree***, *U Welp,* Argonne National Laboratory; *K Kihlstrom,* University of Illinois at Chicago; *A Koshelev,* Argonne National Laboratory; *A Glatz,* Northern Illinois University; *I Sadovskyy, W Kwok,* Argonne National Laboratory **INVITED**

We introduce a new approach for rational design of superconducting critical currents, using time-dependent Ginzburg-Landau simulation to predict the critical current produced by an arbitrary mixed pinning landscape. Time dependent Ginzburg-Landau simulations automatically take into account vortex flexibility, the variation of coherence length with temperature and field, the mutual interaction of vortices and the interaction of vortices and defects. Core pinning by an arbitrary mixed pinning landscape is included by lowering the superconducting condensation energy at points, along lines and within finite nanoscale regions corresponding to specific pinning defects. We show results for several real-world cases that verify predictive ability, outline a program for unfolding the interaction of multiple pinning defects and for maximizing the critical current in targeted temperature and field ranges

*Vortices in High Performance High Temperature Superconductors*, W. K. Kwok et al., Reports on Progress in Physics. 79, 116501 (2016)

*Toward Superconducting Critical Current by Design,* Ivan A. Sadovskyy et al, Advanced Materials 28(23), 4593-4600 (2016)

This work was supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences, as part of the Center for Emergent Superconductivity Energy Frontier Research Center and by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Science.

## Thin Films Division

## Room 21 - Session TF+EM+MI-WeM

## Thin Films for Microelectronics

**Moderators:** Erwin Kessels, Eindhoven University of Technology, the Netherlands, Adrie Mackus, Eindhoven University, Netherlands

8:00am **TF+EM+MI-WeM-1 Electrode Modulated Electric Field Capacitance Nonlinearity in ALD $Al_2O_3$ and $HfO_2$ Metal-Insulator-Metal Capacitors**, *D Austin, K Holden,* ***John Conley, Jr.,*** Oregon State University

Back-end-of-line metal-insulator-metal capacitors (MIMCAPs) require increasing capacitance density ($C_{ox}$) while maintaining low leakage current density ($J_{leak}$). In addition, analog and mixed signal (AMS) applications are particularly sensitive to nonlinearity of capacitance-voltage (CV), empirically characterized by the quadratic voltage coefficient of capacitance, $\alpha_{VCC}$. Scaling of MIMCAPs for AMS applications is increasingly challenging as $C_{ox}$, $J_{leak}$, and $\alpha_{VCC}$ are all inversely proportional to dielectric thickness ($d_{ox}$). Despite its technological importance, the fundamental mechanisms responsible for $\alpha_{VCC}$ are not fully understood. It is well established that the "bulk" dielectric material has a dominant effect, where $\alpha_{VCC}$ increases with increasing dielectric constant and roughly as $1/d_{ox}^2$. However, the influence of the electrode interfaces is not currently understood. Of the few studies that have considered the impact of the electrodes on $\alpha_{VCC}$, most have focused on interfacial layer oxides (ILOs).

In this work, metals with low enthalpy of oxide formation ($\Delta H_{ox}$), are used to examine the influence of the top electrode interface, in the absence of a significant ILO, on the CV nonlinearity of TaN bottom electrode MIMCAPs with various thickness ALD $HfO_2$ and $Al_2O_3$. If non-linearity is purely a bulk effect then normalizing for $d_{ox}$, one would expect that the *electric field* coefficient of capacitance ($\alpha_{ECC}$) should be independent of $d_{ox}$. Instead, we find that $\alpha_{ECC}$*decreases* with decreasing $d_{ox}$, indicating either an ILO or the direct influence of the interface. A plot of capacitive equivalent thickness vs. optical thickness rules out an ILO. For Au, Ag, Pd, and Ni, $\alpha_{ECC}$ increases with increasing $d_{ox}$, saturating for thick oxides. It has been proposed that for positive $\alpha_{VCC}$ materials ($C_{ox}(V)$ increases with voltage), electrostriction and Maxwell stress lead to a vertical compression of the oxide under applied fields that results in increased capacitance. We further propose that the oxide must expand horizontally to maintain volume. This expansion results in compressive stress in the oxide and tensile stress in the metal, concentrated near the interface. The electrode then serves to inhibit the lateral expansion of the dielectric, reducing overall $\alpha_{ECC}$. Indeed $\alpha_{ECC}$ of 10 nm oxides was found to increase roughly linearly with increased oxide/metal % lattice mismatch. As thinner oxides are used to achieve higher $C_{ox}$, the metal electrodes exert influence over a greater % of the oxide thickness, increasing the electrode importance and its impact on nonlinearity.

New understanding of the impact of electrodes on $\alpha_{ECC}$ should aid in rapid optimization of low $\alpha_{ECC}$ MIMCAPs.

8:20am **TF+EM+MI-WeM-2 Difference of the Hysteresis in Capacitance-voltage Characteristics of ALD-$Al_2O_3$ MIS Capacitors on Si and GaN Substrate**, ***Masaya Saito***, *T Suwa, A Teramoto,* Tohoku University, Japan; *T Narita,* Toyota Central R&D Labs. Inc., Japan; *T Kachi,* Nagoya University, Japan; *R Kuroda, S Sugawa,* Tohoku University, Japan

We evaluated the difference of hysteresis in capacitance-voltage(C-V) characteristics of ALD-$Al_2O_3$ MIS capacitors for different semiconductors. N-type Cz-Si and n-type GaN wafers which had the bandgap energies of 1.12 and around 3.4 eV, respectively, were used as semiconductor layers for MIS structures. N-type Si wafer was doped with P of $5\times10^{14}$ cm$^{-3}$. The upper layer (2 µm) of n-type GaN wafer was doped with Si of $5\times10^{16}$ cm$^{-3}$ using a metal-organic vapor phase epitaxy. As the gate insulator layers of the MIS structures, the 10 nm-thick $Al_2O_3$ films were formed by the Atomic Layer Deposition (ALD) using $Al(CH_3)_3$ and $H_2O$ at 75 $^oC$, followed by the formation of aluminum as the gate electrodes. MIS capacitors were irradiated by the light of white LED to only before the voltage sweeps of C-V measurements at -3 V followed by the voltage sweeps of -3 à 3 V and 3 à -3 V without irradiation.

We observed that the clockwise hysteresis in the case of Si gradually decreased as increasing the time of measurement. On the contrary, the hysteresis in the case of GaN was also clockwise and drastically decreased at the second measurement. It is considered that this difference was caused by the difference of bandgap energies between Si and GaN. In the case of Si, some electrons (holes) injected from Si substrate were trapped to the state near the $Al_2O_3$/Si interface when the positive (negative) bias was applied to gate electrode. When applying the subsequent negative (positive) bias, most of these charges were released because the bandgap energy of Si is small. In the case of GaN, most of these charges trapped to the state near the $Al_2O_3$/GaN interface were not released within the measurement time because of the interface states far from the both band edges owing to the larger bandgap energy of GaN. Therefore, the different hystereses for their MIS capacitors were probably caused by the difference that the trapped charges to the state in the bandgap were released in the case of Si but not released in the case of GaN.

Acknowledgement:

This research is supported by the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan, through its "Program for research and development of next-generation semiconductor to realize energy-saving society. This work was carried out at fluctuation free facility of New Industry Creation Hatchery Center, Tohoku University.

8:40am **TF+EM+MI-WeM-3 Monolithic Integration of C-type Erbium Oxide on GaN(0001) by Atomic Layer Deposition***, **Pei-Yu Chen**, A Posadas,* The University of Texas at Austin*; S Kwon, Q Wang, M Kim,* The University of Texas at Dallas*; A Demkov, J Ekerdt,* The University of Texas at Austin

Motivated by the need for faster device speed, the industry is considering compound semiconductors, such as gallium nitride (GaN) in the III-V family of materials, which have higher electron mobility than silicon. To passivate the nitride surfaces and enable GaN-based electronic devices, a high quality and thermally stable dielectric layer material is required. Recently, rare earth sesquioxides have received attention due to their electrical properties, thermal and chemical stability, and relatively high dielectric constant [1]. Using atomic layer deposition (ALD) with erbium tris(isopropylcyclopentadienyl) $[Er(^iPrCp)_3]$ and water, crystalline cubic (C-type) $Er_2O_3$ is successfully grown on GaN at 250 °C for the first time. ALD enables the conformal deposition of $Er_2O_3$ film on GaN and features a stable growth rate of 0.82 Å/cycle in this work. *In-situ* x-ray photoelectron spectroscopy is used to determine film composition and *in-situ* reflection high-energy electron diffraction is used to verify the surface order and the film crystallinity at various stages in the growth process. The cubic structure of $Er_2O_3$ is confirmed by a combination of both out-of-plane and in-plane X-ray diffraction (XRD). The orientation relationships between C-$Er_2O_3$ film and GaN substrate are C-$Er_2O_3$(222) || GaN(0001), C-$Er_2O_3$(-440) || GaN(11-20), and C-$Er_2O_3$(-211) || GaN(1-100). The out-of-plane C-$Er_2O_3$(222) XRD peak shifts as a function of film thickness indicating a slight change in *d*-spacing caused by the presence of strain at the interface as shown in **Fig. 1(a)(b)**. The observed tensile strain results from the lattice mismatch between GaN and $Er_2O_3$. As the film thickness increases, the C-$Er_2O_3$ becomes more relaxed. In-plane XRD also displays peak shifts with opposite trend from the out-of-plane scan as expected. Scanning transmission electron microscopy (STEM) is used to examine the microstructure of C-$Er_2O_3$ and its interface with GaN and is in excellent agreement with the simulated atomic positions (**Fig. 1(c)**). An interfacial layer consisting of 1-3 atomic-layers is observed by STEM. The electron energy loss spectroscopy (EELS) profiles for Ga, Er, O, and N suggest partial oxidization of GaN at the interface. Overall, this work demonstrates a low temperature, all-chemical process for the growth of crystalline C-$Er_2O_3$ on GaN by ALD.

[1] R. Dargis, A. Clark, F. E. Arkun, T. Grinys, R. Tomasiunas, A. O'Hara, and A. A. Demkov, " Monolithic integration of rare-earth oxides and semiconductors for on-silicon technology," *J. Vac. Sci. Technol. A*, 32, 041506 1-8 (**2014**).

9:00am **TF+EM+MI-WeM-4 High-Performance p-Type Thin Film Transistors Using Atomic-Layer-Deposited SnO Films***, S Kim, I Baek, J Pyeon,* Korea Institute of Science and Technology, Republic of Korea*; T Chung, J Han,* Korea Research Institute of Chemical Technology, Republic of Korea*; **SeongKeun Kim**,* Korea Institute of Science and Technology, Republic of Korea

Since the report of thin film transistors (TFTs) utilizing an amorphous oxide semiconductor of the In–Ga–Zn–O system exhibiting high electron mobility by the Hosono group, considerable efforts have been dedicated to implement these TFTs for emerging applications including flat-panel and flexible displays. Compared with the great progress and success regarding n-type oxide semiconductors, the current status of the development of p-type oxide semiconductors remains far behind.

SnO is a promising p-type oxide with relatively high hole mobility. The low formation energy of Sn vacancies and the more dispersed VBM resulting from hybridization of oxygen 2p and Sn 5s orbitals allow the p-type conduction of SnO. One critical challenge for high-performance SnO TFTs is the instability of the SnO phase. SnO is less stable than $SnO_2$, indicating the difficulty of growth of SnO.

Here, we demonstrate high-performance p-type TFTs with a single phase SnO channel layer grown by atomic layer deposition (ALD). The performance of the SnO TFTs relies on hole carriers and defects in SnO and near the back-channel surface of SnO as well as the quality of the gate dielectric/SnO interface. The growth of SnO films at a high temperature of 210 °C effectively suppresses the hole carrier concentration, leading to a high on-current/off-current ($I_{on}/I_{off}$) ratio. In addition, the SnO films grown at 210 °C achieve high field effect mobility ($\mu_{FE}$) compared with the SnO films grown at lower temperatures because of their large grain size and lower impurity contents. However, the SnO films grown at 210 °C still contain defects and hole carriers, especially near the back-channel surface. The post-deposition process – back-channel surface passivation with ALD-grown $Al_2O_3$ followed by post-deposition annealing at 250 °C – considerably alleviates the defects and hole carriers, resulting in superior TFT performance ($I_{on}/I_{off}$: $2\times10^6$, subthreshold swing: 1.8 Vdec$^{-1}$, $\mu_{FE}$: ~ 1 cm$^2$V$^{-1}$s$^{-1}$). We expect that the SnO ALD and subsequent process will provide a new opportunity for producing high-performance p-type oxide TFTs.

9:20am **TF+EM+MI-WeM-5 Recent Progresses of Atomic Layer Deposited Oxide Semiconductors for Emerging Display Applications***, **Jin-Seong Park**, J Sheng, J Lee,* Hanyang University, Republic of Korea **INVITED**

Recently, transparent amorphous oxide semiconductors have been widely studied for potential use in flat-panel displays, such as active-matrix organic light emitting diodes or liquid crystal displays. Semiconductors based on indium and zinc oxide compounds have been intensively studied since the report on transparent flexible amorphous InGaZnO TFTs based on physical vapor deposition (Hosono group) in 2004.

Among various thin film deposition methods, Atomic Layer Deposition (ALD) has remarkably developed in semiconductor and nano-structure applications since early 1990. The unique properties, including controlling atomic-level-thickness, manipulating atomic-level-composition control, and depositing impurity-free films uniformly, may accelerate ALD related industries and applications in functional thin film markets. One of big and challenging markets, display industry, has been just started to look at the potential to adopt ALD based films in emerging display applications, such as transparent and flexible displays.

In this talk, I will introduce various oxide semiconductor materials such ZnO, SnOx, InOx, ZnSnO, InZnOx, deposited by ALD processes. InOx and SnOx semiconductors were prepared by using a liquid indium precursor ([1,1,1-trimethyl-N-(trimethylsilyl) silanaminato]-indium) and tin precursor (N, N'-tert-butyl-1,1-dimethylethylenediamine stannylene-tin), respectively. The former exhibited highly transparent conducting oxide film property and the latter did the p-type polarity under a water reactant. The Indium oxide films were grown by ALD using as the metal precursor and hydrogen peroxide ($H_2O_2$) as the oxidant. It is found that the electrical properties of the indium oxide layers strongly depend on the ALD growth temperature. At relatively low growth temperatures below 150 $^oC$, indium oxide behaves as a transparent semiconducting oxide. Secondly, amorphous indium zinc oxide thin films were deposited at different temperatures. The ALD process of IZO deposition was carried by repeated supercycles, including one cycle of indium oxide and one cycle of zinc oxide. The IZO growth rate deviates from the sum of the respective $In_2O_3$ and ZnO growth rates at ALD growth temperatures of 150, 175, and 200 °C.

Thin film transistors were fabricated with the ALD-grown IZO thin films as the active layer. The amorphous IZO TFTs exhibited high mobility of 42.1 $cm^2 V^{-1} s^{-1}$ and good positive bias temperature stress stability. Finally, flexible InOx and IZO TFTs on polymer substrates were investigated under various mechanical stress conditions, showing interesting degradations of TFTs. It will be discussed about the following issues.

11:00am **TF+EM+MI-WeM-10 Silicon Nitride Thin Films Grown by Hollow Cathode Plasma-Enhanced ALD using a Novel Chlorosilane Precursor***, **Xin Meng**, H Kim, A Lucero, J Lee, Y Byun, J Kim,* University of Texas at Dallas*; B Hwang, X Zhou, M Telgenhoff, J Young,* Dow Chemical

Plasma-enhanced ALD (PEALD) has become an attractive method of depositing silicon nitride ($SiN_x$) due to its ability to grow high-quality films at low temperatures (≤400°C) for various applications [1]. The use of a chlorosilane precursor, is considered a suitable approach for high-volume manufacturing in the semiconductor industry. Chlorosilane precursors can be applicable to either PEALD $SiN_x$ or thermal ALD $SiN_x$ process. In this work, we have investigated the growth of $SiN_x$ thin films using a novel chlorosilane precursor pentachlorodisilane (PCDS, $HSi_2Cl_5$)(synthesized by Dow Corning Corporation, vapor pressure ~10 mmHg at 20 °C) in comparison with hexachlorodisilane (HCDS, $Si_2Cl_6$). A home-made PEALD system equipped with a hollow cathode plasma source (Meaglow Ltd.) was used in this study.

We analyzed the growth per cycle (GPC) and refractive index (R.I.) as a function of the silicon precursor or plasma exposure time, deposition temperature and plasma power. We also investigated the wet etch rate (WER) in dilute hydrochloric acid as a function of the hydrogen content determined by Fourier Transform Infrared Spectrometry (FTIR), and film density determined by X-ray reflectivity (XRR). Using an $N_2/NH_3$ plasma, saturated growth behavior was demonstrated by PCDS and HCDS with a precursor exposure of $\sim 3\times 10^5$ L. GPC was nearly independent of both deposition temperature and RF power, within the investigated regime. Compared to HCDS, PCDS demonstrated approximately 20–30% higher GPC under the same process condition while maintaining comparable WER.

In addition, it was found that the films with higher hydrogen content had a general tendency to have a higher WER while the films with a higher density or higher R.I. tended to have a lower WER. The oxygen content of the bulk $SiN_x$ films determined by ex-situ X-ray photoelectron spectroscopy (XPS) was approximately 3~5 at. % and didn't have a direct correlation with the WER. Furthermore, MIM capacitors (Al/$SiN_x$/degenerated Si) using PEALD $SiN_x$ films grown with PCDS were fabricated. The capacitors exhibited excellent electrical properties, such as a low leakage current density of $10^{-9}$–$10^{-10}$ A/$cm^2$ at 3 MV/cm, and a high breakdown electric field ~13 MV/cm.

[1]. Meng, X.; Byun, Y.-C.; Kim, H.; Lee, J.; Lucero, A.; Cheng, L.; Kim, J., "Atomic Layer Deposition of Silicon Nitride Thin Films: A Review of Recent Progress, Challenges, and Outlooks," Materials, 9 (12), 1007 (2016)

11:20am **TF+EM+MI-WeM-11 Removal of Charge Centers in Hafnia Films by Remote Plasma Nitruration***, **Orlando Cortazar-Martínez**, J Torres-Ochoa, C Gomez-Muñoz, A De Luna-Bugallo, A Herrera-Gomez,* CINVESTAV-Unidad Queretaro, Mexico

We investigated the effect of soft nitridation on the electrical properties of hafnia-based MOS capacitors. Starting from a cleaned Si (100) wafer a 2 nm of $HfO_2$ thin film is grown by ALD using tetrakis (dimethylamido) hafnium(IV) and water type I as precursors. The growth was performed at a temperature of 250 °C with a 20 sccm flow of ultra-high purity nitrogen (UHP-N). Hafnium oxide soft nitridation was performed by a remote plasma (Litmas) using a power of 2500 W, a substrate temperature of 500 °C, the ultra-high purity nitrogen flow was set at 140 sccm and the working pressure is fixed at $3.5\text{x}10^{-2}$ Torr. A 300 nm titanium nitride (TiN) layer is deposited in-situ after nitration in a sputtering system, avoiding undesired contamination. Finally, MOS capacitors were defined using photolitography and etching process.

Capacitance vs voltage measurements characterization was carrying out at different frequencies (1 kHz to 1 MHz). MOS capacitors before nitriding shows a decreasing value in their accumulation capacitance when the frequency is increased. This behavior is attributed to the defects states located inside the oxide layer[1]. In contrast, MOS capacitors measured after nitriding barely shows dispersion in their accumulation regime as the frequency was varied. Also, it can be noted that the threshold voltage remains unchanged.

Films thickness and composition were characterized by ARXPS[2]. The initial thickness and composition were 20.7 Å and $HfO_{2.09}$. After nitridation the thickness changed to 19.8 Å with a composition of $HfO_{1.4}N_{0.48}$. XPS spectra show that the N 1s peak observed at 396.8 eV is associated with the N-Hf bond[3], showing a robust evidence of a substitutional incorporation of nitrogen species into the $HfO_2$ with a saturation process like the one reported in silicon oxide nitridation[4]. Results can be correlated with the soft nitridation process used during fabrication with the remote plasma in which the substitutional nitrogen to oxygen interchange in the $HfO_xN_y$ films keeping the tetrahedral structure from the ALD hafnium as the same as the original but decreasing the amount of the defect states inside the oxide layer.

[1] A. Herrera-Gómez, A. Hegedus, and P.L. Meissner, Appl. Phys. Lett. 81, 1014 (2002).

[2] P.-G. Mani-Gonzalez, M.-O. Vazquez-Lepe, F. Espinosa-Magaña, and A. Herrera-Gomez, J. Vac. Sci. Technol. A Vacuum, Surfaces, Film., vol. 31, no. 1, p. 010601, 2013.

[3] K.-S. Park, K.-H. Baek, D.P. Kim, J.-C. Woo, L.-M. Do, K.-S. No, Appl. Surface Science 257, 1347, 2010.

[4] A. Herrera-Gómez, A. Hegedus, and P.L. Meissner, Appl. Phys. Lett. 81, 1014 (2002).

11:40am **TF+EM+MI-WeM-12 Seam-free Bottom-up Filling of Trenches with $HfO_2$ using Low Temperature CVD***, **Tushar Talukdar**, W Wang, E Mohimi, G Girolami, J Abelson,* University of Illinois at Urbana-Champaign

Filling a deep structure is always a transport-reaction problem, one that is sensitive to the geometry of the structure. For example, with parallel sidewalls, a conformal process can mostly fill the structure, but as film growth diminishes the width of the remaining opening, the AR rises towards infinity; under that condition, no process can eliminate the "seam" in the center. We have shown, using both diffusion and molecular transport models, that a V-shape with an outwards taper (e.g., 3° or more) is needed for conformal coating to work [1]. The other alternative is to develop a process in which film growth is faster at the bottom of the structure: a *superconformal* process in which the growth rate increases progressively with depth. We previously demonstrated a superconformal process for MgO based on (i) a competition for surface adsorption sites between precursor and water co-reactant, and (ii) a large ratio in diffusivity between the high-mass precursor and low-mass water [2].

Here, we attempt to develop superconformal growth of $HfO_2$ from tetrakis dimethylamido hafnium (TDMA-Hf) based on our previous method for MgO. We choose the TDMA-Hf precursor because it affords excellent film quality in ALD, e.g., $HfO_2$ for gate dielectrics. However, the reaction kinetics of this precursor with water as the co-reactant differ strongly from the competitive adsorption model that is the basis for superconformal MgO deposition. Instead, the film growth rate is nearly independent of precursor flux and increases almost linearly with water flux.

For $HfO_2$, we therefore introduce a new approach in which water is injected in a forward-directed flux through a tube aligned with the trench axis. Water is transported ballistically to the trench bottom, where it partially reflects and creates a *virtual source at the trench bottom*. At the same time, the coating conditions are nearly conformal. The combination of a virtual source at the bottom and nearly conformal growth affords a V-shaped profile and excellent filling characteristics. We also introduce a simple kinetic model that predicts the fill profile based on the measured growth rate kinetics.

A limitation to this method is that rapid film growth also occurs on the exposed top surfaces. For a structure with parallel sidewalls, this tends to narrow the opening such that pinch-off can occur prior to complete fill. One solution is to use a structure with an outwards taper to the sidewalls. Another potential solution is to suppress growth at the trench opening using an inhibitor, which we will demonstrate.

1. W. B. Wang and J. R. Abelson, JAP **116**, 194508 (2014)
2. W. B. Wang *et al.*, JVST A **32**, 051512 (2014)

12:00pm **TF+EM+MI-WeM-13 Low-κ Organosilicon Thin Films Deposited by iCVD for Electrical Insulation of Through Silicon Vias***, **Mélanie Lagrange**, C Ratin, M Van-Straaten, C Ribière, T Mourier, V Jousseaume,* CEA-Leti, France

3D integration is considered as an attractive technological route to fabricate cost-effective, high-performance products with reduced size.[1] This technology is based on the use of Through Silicon Vias (TSV), which are vertical connections between electronic components. One of the key steps in TSV fabrication is their electrical insulation from the Si substrate. Depending on the TSV integration scheme used, the allowed thermal budget is limited. For instance, via-middle and via-last integrations need process temperatures lower than 400°C and 200°C, respectively. Moreover, considering the high Aspect Ratio (AR ≥ 10) required by the TSV-middle integration, a highly conformal deposition technique is needed.

Initiated Chemical Vapor Deposition, iCVD, is a low-energy and solvent-free polymer film fabrication process. It is able to deposit solid materials with high step coverage of deep blind features on low-temperature substrates. In the last decade, this versatile method has enabled the deposition of numerous types of polymers, including organosilicons (OSi)[2]. OSi polymers are low-κ materials having shown to be useful in a broad range of applications, including insulation layers in electronic devices.[3]

In this study, dielectric thin films were deposited from vinyl-based OSi precursors using iCVD. The impact of different process conditions on deposition rate, chemical composition and electrical properties of the films have been investigated. Thin films deposited at low temperature, typically < 60°C, can present low dielectric constants (< 3) without the need of any post-deposition treatment. However the films have to face 400°C thermal budget from BEOL process in via-middle integration, therefore a need for sample stabilization emerged. The impact of thermal or UV-assisted annealing on the films properties was investigated in order to understand the thermal stability of the materials and extrapolate their behavior during TSV fabrication and its integration in a full device fabrication flow (BEOL and Back side process). A study of the step coverage achieved by iCVD-deposited thin films in 10*100 µm TSV was performed. It shows that iCVD is promising to deposit materials with high conformity in high AR TSV. Finally, the integration of these OSi polymers in functional TSV, using a standard metallization process on 300 mm wafers, is presented.

The OSi films depositions were processed in a vertical flow reactor, under a collaboration with Kazuya Ichiki, Bruce Altemus and Jacques Faguet, at TEL Technology Center, America.

[1] Gambino et al., *Micro. Eng.* **135** (2015)

[2] Wang et al., *Adv. Mater.* (2017)

[3] Chen et al., *Annu. Rev. Chem. Biomol. Eng.***7** (2016)

## 2D Materials Focus Topic
## Room 16 - Session 2D+EM+MN+NS-WeA

### 2D Device Physics and Applications

**Moderator:** Humberto Gutierrez, University of South Florida

2:20pm **2D+EM+MN+NS-WeA-1 Capacitance-voltage Characteristics of Graphene-gate MOS Devices: The Effect of Graphene Quantum Capacitance**, ***Ruixue Lian***, *A Ural,* University of Florida

There has been significant research interest in graphene for electronics applications, due to its good electrical conductivity, high optical transparency, mechanical flexibility, and two-dimensional structure. However, the potential of graphene as a channel material replacing silicon is limited due to the absence of a bandgap. On the other hand, graphene is an excellent candidate as a transparent, conductive, and flexible electrode for electronic and optoelectronic devices.

Unlike conventional metals, whose Fermi level is typically pinned at the surface, the Fermi level and hence workfunction of graphene can be tailored by electrostatic gating, chemical doping, or surface engineering. As a result, graphene is also a promising candidate as the gate electrode in metal-oxide-semiconductor (MOS) devices, particularly when transparency or workfunction tunability is a requirement.

In real graphene sheets, charged impurities cause electron-hole puddles and random local electrostatic potential fluctuations (statistically described by a Gaussian distribution), which leads to a modified density of states (DOS). In this work, using this modified DOS, we numerically compute the quantum capacitance of graphene as a function of the graphene electrostatic potential at different temperatures and strengths of the potential energy fluctuations. We compare the exact results to various approximations made in the literature when fitting experimental data. We find that the largest discrepancy between the exact results and the approximations occurs near the Dirac point.

In capacitance-voltage (C-V) characterization of graphene-gate MOS devices, what is measured is not the quantum capacitance versus the graphene potential, but the total gate capacitance versus the gate voltage. We numerically compute the gate voltage as a function of the graphene potential and the resulting C-V characteristics at different temperatures, strengths of the potential energy fluctuations, and equivalent oxide thicknesses. We also consider the effect of series and parallel parasitic impedance to the overall shape of the C-V curves. Furthermore, we numerically compute the full C-V characteristics at different values of the equivalent oxide thickness, silicon doping density, and Dirac voltage of graphene. Finally, we fit our recent experimental C-V data with these theoretical calculations to extract the strength of the potential energy fluctuations and the parasitic impedances.

These results provide important insights into the effect of the graphene quantum capacitance on the C-V characteristics of MOS devices and the potential of graphene as a gate electrode in future MOS technology.

2:40pm **2D+EM+MN+NS-WeA-2 *in-situ* Electrical Characterization of Surface Functionalization and Gate Dielectric Deposition Processes on 2D Transition Metal Dichalcogenides Transistors**, ***Antonio T. Lucero***, *J Lee, L Cheng, H Kim, S Kim, J Kim,* University of Texas at Dallas

Two-dimensional transition metal dichalcogenide (TMD) materials are a subject of intense research for use as future, low-power semiconductors. The successful fabrication of TMD based transistors requires a scalable dielectric deposition process. Atomic layer deposition (ALD) is commonly used to grow high-k gate dielectrics, though deposition of thin, pin-hole free dielectrics is challenging due to the chemically inert basal plane of most TMD materials. To overcome this limitation, surface functionalization processes have been developed to improve ALD nucleation.

In order to elucidate the effects of surface functionalization and subsequent ALD on the electrical characteristics of TMD transistors we use an *in-situ* electrical characterization system to measure the electrical properties of TMD transistors at various steps during the deposition process. $MoS_2$ backgated transistors are loaded into an ultra-high vacuum (UHV) cluster tool where samples can be transferred under UHV conditions between various chambers. The cluster tool is equipped with a thermal ALD chamber, a hollow cathode plasma enhanced ALD chamber, a plasma enhanced chemical vapor deposition chamber, and a UHV electrical probe station. Results for ozone, nitrogen radical, and nitrogen plasma functionalization will be presented. The effect of surface dipoles, precursor adsorption and coverage, and nucleation during the ALD process will be discussed as they relate to the electrical characteristics of the device.

This work was supported by the SWAN Center, a SRC center sponsored by the Nanoelectronics Research Initiative and NIST, and by NRF (No. 2015M3D1A1068061) in Korea. We thank TMEIC for providing the ozone generator and nitrogen radical generator used in this work.

3:00pm **2D+EM+MN+NS-WeA-3 High-K Gate oxide by Low Temperature ALD Technique for 2D Materials and Inert Metal Surfaces**, ***Il Jo Kwak***, University of California at San Diego; *J Park,* University of California at San Diego, Republic of Korea; *S Fathipour, A Seabaugh,* University of Notre Dame; *C Pang, Z Chen,* Purdue University; *A Kummel,* University of California at San Diego

2D materials such as TMDs(Transition Metal Dichalcogenides), Graphene and BN have attracted great attention as new channel materials for future devices due to their excellent electronic and optical properties. For such devices, sub nanometer thick and defect free gate oxide is an essential part. However, due to the inert surface of the materials, high K oxide such as $Al_2O_3$ and $HfO_2$ selectively nucleates on defect sites or step edges. Therefore, for successful integration, preparation of uniform and insulating gate oxides are a matter of importance. In this study, $Al_2O_3$ was deposited on 2D materials surface by low temperature ALD using trimethylaluminum(TMA) and $H_2O$ without any seeding layer or surface treatments. Using short purge time between two precursor pulses at 50C, a CVD component was induced to provide uniform nucleation sites on the surface. The CVD component generates subnanometer AlOx particles[s1] [file:///C:/Users/kwak1/Downloads/2017_AVS_abstract_bilayer_oxide.docx#_msocom_1] on the surface which provide uniform nucleation sites. In order to obtain lower EOT layer, 10 cycles of $Al_2O_3$ ALD was deposited at 50C as a seeding layer and 40 cycles of $HfO_2$ ALD was deposited with Tetrakis(dimethylamido )hafnium (TDMAH) and $H_2O$ at 250C. The same oxide was deposited on a SiGe substrate to compare the oxide characteristics. After ALD, MOSCAPs were fabricated to measure electrical properties. AFM measurement revealed that uniform and defect free oxide layers were nucleated on the surfaces. Capacitance-voltage measurement showed that Cox of the bilayer oxide was 2.5 uF/cm2 and the gate leakage current of the oxide was about $10^{-5}$ A/cm$^2$ which was comparable to the oxide on a SiGe substrate. Identical bilayer oxide layer was deposited on a dual gated $WSe_2$ FETs . Top gate oxide leakage of the device was about $10^{-6}$ A/ cm2. In order to assess the quality of the oxide, a benchmarking study of current density versus EOT of 2D semiconductor FET devices and Si based devises was investigated. The study showed that record-low EOT (1.2 nm) and leakage current ($10^{-8}$ μA/ μm$^2$) comparable to the best Si devices with $La_2O_3$ gate oxide by Iwai *et al* was achieved by the WSe2 FET. This technique was also applied to initiate nucleation[s2] [file:///C:/Users/kwak1/Downloads/2017_AVS_abstract_bilayer_oxide.docx#_msocom_2] on inert metal surfaces which are important for logic memory devices including selectors. Using the bilayer oxide, insulating oxide was prepared on Au electrodes of a MOSFET device. The leakage current of the oxide was as low as $10^{-7}$ A/ cm$^2$.

3:20pm **2D+EM+MN+NS-WeA-4 Exploration and Comparison of Optoelectronic Properties of $MoS_2$ Monolayers with Multilayer Flakes and $Mo_xW_{1-x}S_2$ Ternary Compounds**, ***Sourav Garg***, *J Waters, A Mollah, S Kim, P Kung,* University of Alabama

2D transition metal dichalcogenide (TMDC) semiconductors, including $MoS_2$, $WS_2$, and more recently ternary compounds, exhibit exceptional structural, electrical and optical properties that make these materials of great interest for nano-optoelectronic devices. For example, unlike graphene, TMDCs have a bandgap, which has the remarkable characteristic of becoming direct when the material is in monolayer form, while it is indirect when the material is composed of multiple layers.

Here, we report the synthesis of monolayer $MoS_2$, $WS_2$, ternary $Mo_xW_{1-x}S_2$ ternary compounds and $MoS_2$/$WS_2$-based heterostructures, by chemical vapor deposition (CVD) process at temperatures in the range 950-1000 C, without the use of seeds to avoid contamination. The material was extensively characterized using micro-Raman spectroscopy, micro-photoluminescence, and electron microscopy.

Using such large area CVD grown materials, large-area $MoS_2$ photoconductive detector devices were fabricated using conventional photolithography to realize of interdigitated metal fingers. The electrical and spectral photoresponse from monolayer and multilayer $MoS_2$ have been compared, in terms of responsivity and specific detectivity. The monolayer devices exhibited high photoconductive gain and detectivity near $10^{12}$ Jones, which was also found to be higher than in the case of multilayer $MoS_2$ devices. The rise and decay time of passivated monolayer devices was investigated and shown to be much faster than the unpassivated devices.

4:40pm **2D+EM+MN+NS-WeA-8 Dielectric Properties of Carbon Nanomembranes prepared from aromatic Self-Assembled Monolayers investigated by Impedance Spectroscopy***, **Paul Penner**, E Marschewski, X Zhang,* Bielefeld University, Germany*; T Weimann, P Hinze,* Physikalisch-Technische Bundesanstalt, Germany*; A Beyer, A Gölzhäuser,* Bielefeld University, Germany

Carbon nanomembranes (CNMs) are two-dimensional materials made by cross-linking self-assembled monolayers (SAMs) of aromatic molecules via low energy electron irradiation. Previous study of molecular junction incorporating SAMs and CNMs of oligophenyl thiols has been carried out by using conical eutectic Gallium-Indium (EGaIn) top-electrodes[1] and conductive probe atomic force microscopy (CP-AFM). Here we investigate the dielectric properties of pristine SAMs and CNMs with an EGaIn top electrode by impedance spectroscopy. Analysis and comparison of the tunneling resistance and capacitance density of pristine and cross-linked SAMs revealed a thickness dependent capacitance associated with the monolayer as well as a thickness independent capacitance. We adopted an equivalent circuit to take into account the contribution of the interfacial capacitance as well as the oxide layer of the EGaIn top electrode. The obtained tunneling decay constant remains unaffected after electron irradiation, which exhibits a value of about 0.5 $Å^{-1}$ for both systems. A determination of dielectric constants of SAMs and CNMs from the impedance spectra will also be analyzed and discussed. Furthermore we characterize stacks of CNMs sandwiched with graphene and other 2D materials.

[1] P. Penner, X. Zhang, E. Marschewski, et. al, J Phys Chem C 2014, 118, 21687.

5:00pm **2D+EM+MN+NS-WeA-9 2D Crystals for Next-Generation Ultra Energy-Efficient Electronics***, **Kaustav Banerjee**,* University of California at Santa Barbara **INVITED**

I will highlight the prospects of two-dimensional (2D) materials for innovating energy-efficient transistors, sensors, and interconnects targeted for next-generation electronics needed to support the emerging paradigm of the *Internet of Things*. More specifically, I will bring forward a few applications uniquely enabled by 2D materials and their heterostructures that have been demonstrated in my lab for realizing ultra-energy-efficient electronics. This will include the world's first 2D-channel band-to-band tunneling transistor that overcomes a fundamental power consumption challenge in all electronic devices since the invention of the first transistor in 1947 (Nature 2015), as well as a breakthrough interconnect technology based on doped-graphene-nanoribbons, which overcomes the fundamental limitations of conventional metals and provides an attractive pathway toward a low-power and highly reliable interconnect technology for next-generation integrated circuits (Nano Letters 2016). I will also bring forward a new class of ultra-sensitive and low-power sensors as well as area-efficient and high-performance passive devices, both enabled by 2D materials, for ubiquitous sensing and connectivity to improve quality of life.

## Electronic Materials and Photonics Division
## Room 14 - Session EM+2D+MI+MN-WeA

## Materials and Devices for Quantum Information Processing

**Moderators:** Rachael Myers-Ward, U.S. Naval Research Laboratory, Steven Vitale, MIT Lincoln Laboratory

2:20pm **EM+2D+MI+MN-WeA-1 Controlling the Valley Degree of Freedom in 2D Transition Metal Dichalcogenides***, **Tony Heinz**,* Stanford University / SLAC National Accelerator Laboratory **INVITED**

Monolayer transition metal dichalcogenide crystals in the $MX_2$ family with M = Mo, W and X = S, Se have been shown to provide attractive possibilities for access to the valley degree of freedom both optically and through the valley Hall effect. In this paper we will summarize recent advances in the electrical and optical control of the valley degree of freedom in this class of materials.

The optical selection rules in the transition metal dichalocogenide monolayers permit selective creation of excitons in either the K or K' valley through the use of circularly polarized light. Excitons consisting of coherent superpositions of both valleys can also be produced through excitation with linearly polarized light. While these results have already been demonstrated experimentally, to date there has been no report of an approach to *manipulate* the valley exciton pseudospin after its creation. In this paper we present our recent use of the optical Stark effect to dynamically modify the valley pseudospin. The approach is based on selectively altering the energy of one valley vis-a-vis the other through application of a sub-gap optical pulse with circular polarization. This perturbation leads to a rapid rotation of the exciton valley pseudospin, as revealed by a change in the polarization state of the exciton emission.

In a second line of investigation, we have applied to spin-valley Hall effect in transition metal dichalocogenide monolayers to produce spatially separated regions with enhanced valley (and spin) populations. This is achieved by running a current through a hole-doped monolayer and relying on the anomalous velocity terms to separate the holes spatially. The resulting spin-valley spatial profile has been directly imaged on the micron scale and characterized using measurements based on the optical Kerr effect. The magnitude of this spin-valley imbalance and its dependence on doping and bias fields have been investigated and compared with theoretical predictions.

3:00pm **EM+2D+MI+MN-WeA-3 VOI-based Valleytronics in Graphene***, **Yu-Shu Wu**,* National Tsing-Hua University, Taiwan, Republic of China **INVITED**

Electrons in gapped graphene carry a unique binary degree of freedom called valley pseudospin, in association with the two-fold valley degeneracy at the Dirac points (K and K') of Brillouin zone. Such pseudospin carries an intrinsic angular momentum and responds to external electromagnetic fields in ways similar to those of an ordinary electron spin [1,2]. We examine the response and address the important issue of valleytronics - the electrical manipulation of valley pseudospin. A unified methodology called VOI based valleytronics will be presented, which exploits the valley-orbit interaction (VOI) between an in-plane electric field and a valley pseudospin for the implementation of valleytronics. Based on the VOI mechanism, a family of fundamental structures have been proposed with important device functions, such as valley qubits, valley filters, and valley FETs [3]. We will report recent theoretical developments in these structures.

[1] Rycerz et al., Nat. Phys. **3** (2007),172.

[2] Xiao et al., Phys. Rev. Lett. **99**, (2007), 236809.

[3] Wu et al., Phys. Rev. B **84**, (2011), 195463; *ibid* B **86** (2012), 165411; *ibid* B **88** (2013), 125422; *ibid* B **94** (2016), 075407.

4:20pm **EM+2D+MI+MN-WeA-7 Creating Quantum Technologies with Spins in Semiconductors***, B Zhou, **David Awschalom**,* University of Chicago **INVITED**

There is a growing interest in exploiting the quantum properties of electronic and nuclear spins for the manipulation and storage of information in the solid state. Such schemes offer fundamentally new scientific and technological opportunities by leveraging elements of traditional electronics to precisely control coherent interactions between electrons, nuclei, and electromagnetic fields. Although conventional electronics avoid disorder, recent efforts embrace materials with incorporated defects whose special electronic and nuclear spin states allow the processing of information in a fundamentally different manner because of their explicitly quantum nature [1]. These defects possess desirable qualities – their spin states can be controlled at and above room temperature, they can reside in a material host amenable to microfabrication, and they can have an optical interface near the telecom bands. Here we focus on recent developments that exploit precise quantum control techniques to explore coherent spin dynamics and interactions. In particular, we manipulate a single spin in diamond using all-optical adiabatic passage techniques [2], and investigate the robustness of the acquired geometric (Berry) phase to noise as well as novel strategies to overcome traditional speed limits to quantum gating. Separately, we find that defect-based electronic states in silicon carbide can be isolated at the single spin level [3] with surprisingly long spin coherence times and high fidelity, can achieve near-unity nuclear polarization [4] and be robustly entangled at room temperature [5]. Finally, we identify and characterize a new class of optically controllable defect spin based on chromium impurities in the wide-bandgap semiconductors silicon carbide and gallium nitride [6].

[1] D.D. Awschalom, L.C. Bassett, A.S. Dzurak, E.L. Hu and J.R. Petta, Science 339, 1174 (2013).

[2] C. G. Yale, F. J. Heremans, B. B. Zhou, et al., Nature Photonics 10, 184 (2016); B. B. Zhou et al., Nature Physics 13, 330 (2017).

[3] D. J. Christle, A. L. Falk, P. Andrich, P. V. Klimov, et al., Nature Materials 14, 160 (2015); D. J. Christle et al., arXiv:1702.07330 (2017).

[4] A. L. Falk, P. V. Klimov, et al., Physical Review Letters 114, 247603 (2015).

[5] P. V. Klimov, A. L. Falk, D. J. Christle, V. V. Dobrovitski, and D. D. Awschalom, Science Advances 1, e1501015 (2015).

[6] W. F. Koehl et al., Editors Suggestion, Phys. Rev. B 95, 035207 (2017).

5:00pm **EM+2D+MI+MN-WeA-9 Diamond as an Electronic Material: Opportunities and Challenges***, **Steven Vitale**, J Varghese, M Marchant, T Wade, M Geis, T Fedynyshyn, D Lennon, M Hollis,* MIT Lincoln Laboratory

Diamond possesses extraordinary semiconductor properties including carrier mobility, saturation velocity, and thermal conductivity which far exceed those of silicon and essentially all other semiconductor materials. In spite of these incredible qualities diamond has not yet become a mainstream transistor material, for two primary reasons. First, existing small single-crystal substrates have not been able to take advantage of commercial microelectronics processing equipment and growth of wafer-scale single-crystal diamond has not been vigorously pursued. Second, deep donor and acceptor levels in diamond imply that the impurity ionization fraction is quite low at room temperature which results in low carrier density in conventional FET architectures.

However the situation has changed dramatically in the past few years. Plasma-enhanced CVD promises to create large-wafer single-crystal diamond through mosaic or novel catalytic growth.[1] Additionally, the discovery of the diamond surface FET has addressed the problem of low carrier density.[2] Together, these advancements may allow development of practical diamond transistors with unparalleled performance for high-power, high-frequency applications. Many unit process and process integration challenges remain to develop diamond surface FETs into commercial technology. This paper will report on the state of the art in diamond surface FET technology and will examine current unmet needs.

We have developed diamond surface FETs with current densities in excess of 100 mA/mm. This is enabled by a novel surface activation process using a high concentration of $NO_2$ in air to react with a hydrogen-plasma-treated diamond surface. The electron accepting nature of the modified surface abstracts an electron from the diamond, resulting in a 2D hole gas (2DHG) in the diamond. We measure a hole mobility of 30-130 $cm^2/V\text{-}s$ and a repeatable surface resistance of ~ 1.5 kΩ $sq^{-1}$ using this technique. 2DHG formation has been demonstrated using other surface moieties as well, including photoacid radical generators and trinitrotoluene. Pros and cons of these different surface adsorbates will be discussed. The performance of Au, Mo, Pt, Al, Pd, Ti, Cr contacts, as well as combinations of these metals will be presented, with a record-low diamond contact resistance of 0.6 ohm-mm and good ohmic behavior.

[1] M. Schreck, et al, Sci. Rep. 7, 44462 (2017).

[2] M. Kasu, Japanese Journal of Applied Physics 56, 01AA01 (2017).

5:20pm **EM+2D+MI+MN-WeA-10 Studies on Influence of Processing on Optical Characteristics of Electron Irradiated 4H-SiC Nanostructures***, **Shojan Pavunny**,* ASEE Research Fellow at U.S. Naval Research Laboratory*; H Banks,* NRC Research Fellow at U.S. Naval Research Laboratory*; P Klein,* U.S. Naval Research Laboratory*; K Daniels,* NRC Research Fellow at U.S. Naval Research Laboratory*; M DeJarld,* ASEE Research Fellow at U.S. Naval Research Laboratory*; E Glaser, S Carter, R Myers-Ward, D Gaskill,* U.S. Naval Research Laboratory

Spin-coherent single silicon defect centers ($V_{Si}$) in wide bandgap silicon carbide polytypes have recently drawn great research interest for future applications in information technologies such as scalable quantum computing, sensing and metrology. Identification of these deep defects, gaining a thorough knowledge of their characteristics, active control of their concentrations, isolation of single spin defects and understanding the effects of semiconductor processing on their properties are crucial challenges for the realization of SiC based quantum electronic and integrated photonic devices. These color centers coupled to photonic crystal cavities (PCC) have the capability of high efficiency emission of zero phonon lines which can significantly improve the performance of on-chip photonic networks and long-distance quantum communication systems, as compared to conventional solid-state emitters. Here we investigate the impact of fabrication process on the photoluminescence properties of PCCs realized using three techniques: hydrogen implantation to form thin SiC layers on an oxide layer that can be easily etched away to form an air gap under the PCC, wafer bonding and mechanical thinning of the SiC, also on an oxide layer, and selective electrochemical anodization of an n-p epitaxial SiC structure to form an air gap. We also comment upon the impact of electron irradiation for these three fabrication techniques.

5:40pm **EM+2D+MI+MN-WeA-11 Ab Initio Simulations of Point Defects in Solids Acting as Quantum Bits***, **Adam Gali**,* Wigner Research Centre for Physics, Hungarian Academy of Sciences, Hungary **INVITED**

Luminescent and paramagnetic point defects in insulators and semiconductors may realize quantum bits that could be the source of next generation computers and nanoscale sensors. Detailed understanding of the optical and magnetic properties of these defects is needed in order to optimize them for these purposes.

In this talk I show our recent methodology developments in the field to calculate the ground and excited state of point defects and to determine their Auger-rates, hyperfine tensors and electron spin – electron spin couplings, and intersystem crossing rates. We show recent results on the nitrogen-vacancy center in diamond as well as divacancy and other defects in silicon carbide that we have found a very promising alternative to the well-established nitrogen-vacancy center for integration of traditional semiconductor and quantum technologies into a single platform.

## Electronic Materials and Photonics Division
## Room 14 - Session EM+MI+NS+SP+SS-ThM

## Photonics, Optoelectronics, and Light Manipulation

**Moderators:** Yohannes Abate, Georgia State University, Nikolaus Dietz, Georgia State University

8:00am **EM+MI+NS+SP+SS-ThM-1 Evolutionary Design of Multi-functional Optical Metasurfaces***, **Teri Odom**,* Northwestern University **INVITED**

Metasurfaces are an emerging class of flat optics that can manipulate light via subwavelength phase elements. Their 2D structures are usually determined by (1) calculating the phase change required at each location to obtain far-field properties from analytical equations and (2) structuring each building block to produce that wavefront change. However, computational or digital approaches to design metasurfaces based on search heuristics offer advantages in targeting and realizing properties not possible by analytical expressions. This talk will describe an evolutionary approach to design flat lenses based on subwavelength plasmonic building blocks. Our lattice evolution algorithm can achieve desired optical responses by tuning the arrangement of the phase units on a discrete square lattice. We will discuss two different systems with different classes of building units—holes and particles—to realize achromatic lattice lenses at up to three wavelengths and flat lenses in semiconductor plasmonic materials such as titanium nitride. We will describe prospects for scaling the production of these lenses as well as their ability to achieve dynamic optical responses.

8:40am **EM+MI+NS+SP+SS-ThM-3 Dielectric Freeform Metasurfaces for Optical Sensing***, **Arka Majumdar**,* University of Washington, Seattle **INVITED**

The macroscopic volume of optical sensors, such as cameras, often originates from the requirement of having multiple optical elements and thick spherical geometries. In recent years, researchers have made subwavelength optical elements, commonly known as metasurfaces, with an ultra-thin form factor using well-developed semiconductor nano-fabrication technology. In parallel with the progress in such nano-photonic devices, researchers have also made vast improvements in the field of freeform optics. Freeform optics aim to expand the toolkit of optical elements beyond those exhibiting rotational symmetry. Most conventional optical elements have rotational symmetry for manufacturing reasons, but freeform optics emphasizes complex surface geometries, which are difficult to manufacture by traditional means. While both metasurface and freeform optics have progressed substantially in recent years, they have developed independently of one another as their respective research communities are disconnected.

In our work, we demonstrated how metasurface technology can be used for the realization of subwavelength scale freefrom optics, with applications in implantable bio-sensing and potentially in augmented reality systems. I will present some of our recent results on metasurface freeform optics that enable a large depth of focus and a tunable focal length lens. I will also show how these metasurfaces can be used to perform truly colored imaging, by virtue of the extended depth of focus. Finally, I will talk about our ongoing work on metasurface based cavity engineering.

9:20am **EM+MI+NS+SP+SS-ThM-5 Moth eye-based, graded index surface treatments to control reflection and light extraction***, L Chan, C Pynn, P Shapturenka, R Ley, S Denbaars, D Morse, **Michael Gordon**,* University of California at Santa Barbara

This talk will highlight our recent work on bio-inspired surface treatments to control reflection and enhance light extraction at interfaces. An easy, scalable and defect-tolerant surface modification protocol, based on colloidal lithography and plasma etching, was developed to create synthetic 'moth-eye' (ME) anti-reflective structures in different material platforms for photonics and energy applications. Large increases in transmission, bandwidth, and omni-directional response were obtained in Si, Ge, GaAs, ZnS/ZnSe, and CdTe platforms for IR (2-50+ um), with performance better than commercial, interference-based coatings. Effective medium theory, finite difference time domain (FDTD) simulations, and quantitative measurements of transmission, reflection and diffuse scattering were used to understand the ‘photon balance’ of ME films to investigate how optical behavior depends on moth-eye geometry, (dis)order, and pattern fidelity. ME coatings were also implemented in blue-green InGaN/GaN quantum well LED structures on c-plane and semi-polar substrates to enhance light extraction and device efficiency. A 4.8-fold overall enhancement in light extraction (9-fold at normal incidence) compared to a flat surface was achieved using a feature pitch of 2530 nm—performance on par with current photoelectrochemical (PEC) roughening methods. The colloidal lithography roughening technique presented herein is independent of GaN crystal orientation and is therefore applicable to roughening semipolar and nonpolar GaN devices, on which PEC roughening is ineffective.

9:40am **EM+MI+NS+SP+SS-ThM-6 Infrared Surface Plasmon-influenced Interfacial Chemistry of Semiconductor Nanocrystals***, W Hu, **Michael Filler**,* Georgia Institute of Technology

Localized surface plasmon resonances (LSPRs) present exciting opportunities to improve the spatial and temporal control of chemistry at semiconductor surfaces. While the ultraviolet and visible LSPRs supported by metallic nanoparticles are known to impact surface chemistry, heavily-doped semiconductor nanocrystals promise similar capabilities in the near and mid-infrared. Here, we use time-resolved *in situ* infrared spectroscopy to study the influence of mid-infrared LSPRs on a model interfacial process: desorption. We find that the molecular desorption rate for a range of "beacon" molecules (e.g., indole, benzoic acid) on indium tin oxide (ITO) nanocrystals is enhanced by as much as 2x upon illumination with mid-infrared light (~0.6-0.1 eV) at room temperature. The desorption rate is linearly dependent on light intensity, indicating a single photon process. Experiments as a function of LSPR energy, nanocrystal film thickness, and adsorbate concentration provide clues as to the mechanism of the enhancement. Our findings open new avenues to leverage low energy photons for manipulating chemical reactions on the surfaces of heavily-doped semiconductors.

11:00am **EM+MI+NS+SP+SS-ThM-10 Dynamically Tunable Polarization Response in a Si/Au Metamaterial***, **Nicole Pfiester**,* Tufts University*; C Shemelya,* Technische Universität Kaiserslautern, Germany*; D DeMeo, E Carlson, T Vandervelde,* Tufts University

Polarimetry is utilized across many fields, from chemical characterization to classification of astronomical objects to the detection of man-made items. Present technology requires a different filter for each polarization of light you wish to measure. This requires either a cluster of four pixels to differentiate between the polarizations incident on an area, reducing the final image resolution compared to a non-polarized image, or a filter wheel that adds weight and mechanical reliability issues. Metamaterials can be leveraged to design materials with a polarization sensitive response. Application of a bias voltage can further alter the material’s interaction with incident light, resulting in a metamaterial whose response can be tuned dynamically. This technique can be used to create a filter that can be turned on and off for a given polarization. An integrated stack of these filters would allow the measurement of any polarization direction at the full resolution capacity of the detector with the advantages of on-chip integration.

We designed a metamaterial structure that generates a polarization-dependent response in the mid-infrared wavelength range. Off-setting the absorption and transmission peaks for the two polarizations allows equal transmission while the filter is in a static state, or without a bias voltage. The application of a bias changes the metamaterial response and blocks polarized waves parallel to one axis. A thin film semiconductor layer is required to achieve this effect. Previous work utilized thin film gallium arsenide, but poor film quality of the epitaxial layer, with surface roughness on the order of the metamaterial feature size, did not provide sufficient conductivity for an applied bias to impact the light interactions. We will present new results using thin film silicon with a gold nanostructure pattern. A static filter, one that does not require an applied voltage to operate as a polarizing filter, was fabricated to demonstrate the design suitability. We will report on our progress toward a dynamic filter and compare to previous results with III-V films.

11:20am **EM+MI+NS+SP+SS-ThM-11 Imaging Stress Induced Lateral Quantum Barrier Manipulation of Indium Gallium Arsenide Quantum Wells, using Micro-Photoluminescence Spectroscopy***, **Brian Rummel**, M Rimada, S Addamane, G Balakrishnan,* University of New Mexico*; T Sinno,* University of Pennsylvania*; S Han,* University of New Mexico

We have previously demonstrated that a patterned elastic stress field can be used to change the near-surface atomic composition in epitaxial compound semiconductor films.[1] This compositional patterning laterally manipulates quantum barriers within the film in a press-and-print manner, completely eliminating the need for Stranski-Krastanov growth. For the proof-of-concept, the said mechanism was used to diffuse Ge in a SiGe substrate to form regions of Ge-depleted, pure Si surrounded by SiGe. This result opened the door to thermo-mechanically triggered, rewritable circuitry for a wide variety of applications. For the current effort on InGaAs quantum well systems, an array of Si pillars is pressed against a GaAs/$In_{.20}Ga_{.80}As$/GaAs substrate in a mechanical press, and the assembly is heated to elevated temperatures. The applied elastic stress field promotes the diffusion of larger In atoms away from the compressed regions, leaving In-depleted GaAs in localized regions of the quantum well. Careful assembly and design of the Si nanopillar array would controllably define GaAs and InGaAs regions, producing laterally organized quantum structures. Photoluminescence spectroscopy is used to confirm the diffusion of In and compositional variation, based on the wavelength shift of the emission line from the InGaAs quantum well. In this presentation, we will further discuss how micro-photoluminescence imaging can be used to directly image regions of In-enriched regions as well as In-depleted regions found under the elastically compressed areas. This method may allow us to register the compositionally altered regions for addressable circuitry.

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11:40am **EM+MI+NS+SP+SS-ThM-12 Silicon-Based Infrared Photodetectors Enabled by Hot Electrons***, **Seok-Jun Han**, S Han, S Han,* University of New Mexico

Infrared (IR) detectors typically employ low band gap materials, such as InGaAs, InSb, or HgCdTe. However, these materials include elements that are rare, expensive, or toxic. Past research indicates that low-cost, abundant crystalline Si (c-Si) could be used for IR detection when metal electrodes are appropriately nanostructured. In this type of photodetection, the IR with energies below the Si band gap is strongly absorbed by the metal structures. The photoexcited electrons in the metal can then be injected into the conduction band of c-Si before being thermalized, and electric current can be generated. These non-thermalized hot electrons enable the detection of IR light with energies below the c-Si band gap. For efficient transport of electrons in the metal before thermalization, the metal layer should be as thin as approximately the electron mean free path. To induce strong optical absorption in such a thin metal layer, surface plasmon polaritons (SPPs) can be excited at the metal surface. Previous studies on hot electron photodetection utilized small-scale metamaterials or deep trench resonators to have strong resonant absorption of SPPs in thin metal films on c-Si at the desired frequencies. However, these structures had to be fabricated with high precision (e.g., e-beam lithography) because the metal structure size determines resonance. In this study, we pursue a low-cost, manufacturable path, which can tolerate practical fabrication errors. We make use of metal metasurfaces that can be fabricated by scalable, inexpensive techniques and achieve a broad-band IR absorption of over 95% in 15-nm-thick metal films. This unprecedented strong and broad-band absorption is enabled by a new scheme which uses multiple modes of SPPs while the light takes multiple passes within the c-Si substrate. During the passage, light is preferentially absorbed by the thin metal layer that is on one side of the substrate. Absorption on the other side is efficiently eliminated by using a dielectric layer. In our effort, the surface of the c-Si substrate where thin meal film is deposited is structured by a simple optical lithography. The structured surface admits the incident light into the substrate and prevents the light from leaking out of the substrate. In our scheme of multiple light passes, extremely strong resonances are not necessary and fabrication errors would not destroy the optical properties appreciably. In this talk, we will discuss the details of the optical absorption in our scheme. We will also present our experimental results on the electronic characteristics of our hot electron devices.

12:00pm **EM+MI+NS+SP+SS-ThM-13 Low Temperature Wafer Bonding of LTG-GaAs to Si3N4for Terahertz Photoconductive Switch Application***, X Fu,* Illinois Institute of Technology and Argonne National Laboratory*; M Haji-Sheikh, G Westberg, S Ross,* Northern Illinois University*; E Landahl,* DePaul University*; K Attenkofer,* Brookhaven National Laboratory*; **Thomas Wong**,* Illinois Institute of Technology

Integrating GaAs optoelectronic devices with Si- based platforms has attracted much attention and efforts in recent years, as a thin layer of GaAs can exhibitsuperior bulk quality. Wafer bonding, an emerging approach of monolithic integration of GaAs on Si-based substrate, overcomes the lattice mismatch in heterogeneous growth. Several techniques with a post-bonding annealing at temperature exceeding 800°C have been demonstrated to achieve high-energy covalent bonds between III-V compound semiconductors and Si/SiO2systems. However, the elevated temperature bonding process may create not only an inevitable thermal mismatch barrier but also damage the bonding materials. Thus, there is a need for improved technique to integrate GaAs with silicon based devices.

Low temperature grown (LTG) GaAs, which is typically obtained by molecular beam epitaxy (MBE) at temperatures as low as 200°C, offers very attractiveproperties such as ultra-short carrier lifetime, high electron mobility and high resistivity. It is verydesirable for applications such as ultrafast photoconductive switch, high efficiency solar cells and infrared LEDs. Pioneering work has demonstrated techniques to bond LTG-GaAs to Si/ SiO2 at temperature as low as room temperature by means of plasma activation and by wafer bonding under vacuum. However, very few techniques have been developed to bond LTG-GaAs layer to Si3N4 substrate, mainly because Si3N4 is naturally hydrophobic and bonding has been considered unachievable10. The existing Si3N4 bonding techniques employ high temperature fusion of Si3N4 layers or apply a layer of bonding agent such as SiO2.

In this paper, we report a room temperature approach to directly bond LTG-GaAs to Si3N4 by activating the surface of Si3N4 using weak HF acid solution. This method can be implemented on Si3N4 deposited over wide temperature range. Procedures to reduce the bonding voids and improve the bond strength are also described. In an application to utilize the developed method, we implemented this approach to fabricate a photoconductive switch on Si3N4 substrate bonded with LTG-GaAs and validated that the bonded LTG-GaAs retained the electro-optical properties. A THz opticalcross correlation test showed that the photoconductive switch responded swiftly to a femtosecond Ti-Sapphire laser pulse with a resolution of approximately 0.25ps. This wafer bonding method can be integrated with a wide range of microelectronic device fabrication thatrequires the bonding of LTG-GaAs layer with Si3N4.

## Nanometer-scale Science and Technology Division
## Room 19 - Session NS+AS+EM+MI+SP+SS-ThM

### Nanoscale Imaging and Characterization

**Moderators:** Stephane Evoy, University of Alberta, Indira Seshadri, IBM Research Division, Albany, NY

8:00am **NS+AS+EM+MI+SP+SS-ThM-1 Characterizing Optoelectronically-Active Molecules via STM Imaging and Advanced Raman Spectroscopy Techniques***, J Schultz, P Whiteman, Z Porach, **Nan Jiang**,* University of Illinois at Chicago

In response to the ever increasing demand for cleaner, cheaper energy generation, significant efforts have been made to fabricate and characterize materials that can be used for optoelectronic devices. Porphyrins, phthalocyanines, and their derivatives have been involved in many surface studies to investigate their optoelectronic properties for use in organic photovoltaics and other optoelectronic devices, such as organic light-emitting diodes (OLED). Our research take place in a commercial ultrahigh vacuum (UHV) scanning tunneling microscopy (STM) chamber. Molecules were evaporated onto various single crystal substrates at a base pressure of $10^{-10}$ torr. Different surface-supported structures were imaged via STM at sub-molecular resolution, allowing the competition of molecule-substrate and molecule-molecule interactions to be investigated.

In addition to imaging via STM, we also performed spectroscopy experiments in the forms of UHV Tip Enhanced Raman Spectroscopy (TERS), supplementing vital vibrational information at single-molecule spatial resolution. These tools provide a complete picture of the system in question, allowing our lab to answer previously unknown questions regarding the molecule-molecule interactions in order to characterize the molecule's exciton-generating and electron-transferring properties at a fundamental level.

8:20am **NS+AS+EM+MI+SP+SS-ThM-2 BCC to FCC Phase Transition of $Pd_xCu_{1-x}$ at Nanoscale***, **Xiaoxiao Yu**,* Carnegie Mellon University*; A Gellman,* Carnegie Mellon University, W.E. Scott Institute for Energy Innovation

One of the most interesting characteristics of alloy nanoparticles (NPs) is that they can have different phases from those of the bulk. In the bulk phase diagram of $Pd_xCu_{1-x}$, there exists a composition range, $0.35 < x < 0.55$, over which a B2 phase (ordered body centered cubic, CsCl structure) is formed at $T < 873$ K, in spite of the fact that pure Pd and Cu both have face centered cubic (FCC) bulk crystal structures. An experimental methodology has been developed for determining the phase behavior of $Pd_xCu_{1-x}$ size and composition spread nanoparticle (SCSNP) libraries. Spatially resolved X-ray photoemission spectroscopy (XPS) was used to map the Cu 2$p_{3/2}$ core level shifts (CLS) with respect to the value for pure Cu across composition space on the bulk Pd$_x$Cu$_{1-x}$ alloy. The result has shown that the Cu 2$p_{3/2}$ binding energy decreases monotonically with increasing Pd at.% in the FCC phase. There is additional discontinuous CLS over the composition range from 0.35 to 0.55 Pd at.%, where the B2 phase forms. Therefore, the Cu 2$p_{3/2}$ core level binding energy measured by XPS can be used to distinguish between the ordered B2 phase and disordered FCC phase. The Pd$_x$Cu$_{1-x}$ SCSNP library on a Mo substrate was prepared using a rotatable shadow mask deposition tool previously developed by our group. After annealing the Pd$_x$Cu$_{1-x}$ alloy thin film to 700 K, the additional CLS over the composition range, 0.35 < x < 0.55, has been observed at a film thickness > 6 nm, which suggests the formation of B2 phase. However, at a film thickness between 4 – 6 nm, the Cu 2$p_{3/2}$ binding energy decreases monotonically across composition space which suggests that only FCC phase exists for alloy films in this thickness range. Because the FCC phase is more densely packed than the B2 phase, the surface tension in this thickness regime can drive a conversion from the ordered B2 phase back to the randomly distributed FCC solid solution. More interestingly, the additional CLS over the composition range from 0.35 to 0.55 Pd at.% reoccurs at a film thickness < 4 nm, which suggests the formation of B2 phase. This observation is the result of dewetting of the Pd$_x$Cu$_{1-x}$ NPs after heating at 700 K for 30 mins, and the size of dewetting NPs exceeds 6 nm where the close-packed FCC phase is stabilized. Dewetting of Pd$_x$Cu$_{1-x}$ NPs is validated by the appearance of the substrate Mo XPS signal at a film thickness < 4 nm. This comprehensive experimental study of the phase behavior for Pd$_x$Cu$_{1-x}$ alloy NPs will be correlated with their catalytic activity across composition and size spaces to accelerate the development of alloy NPs for catalytic applications.

8:40am **NS+AS+EM+MI+SP+SS-ThM-3 Hybrid Environmental Transmission Electron Microscope: An Integrated Platform for In situ Imaging and Spectroscopies***, **Renu Sharma,*** NIST **INVITED**

Environmental transmission electron microscopes (ETEM) and TEM holders with windowed reaction cells, enable in situ measurements of the dynamic changes occurring during gas-solid and/or liquid-solid interactions. The combination of atomic-resolution images and high spatial and energy resolution has successfully revealed the nucleation and growth mechanisms for nanoparticles, nanowires, carbon nanotubes and the functioning of catalyst nanoparticles. While TEM-based techniques are ideally suited to distinguish between active and inactive catalyst particles and identify active surfaces for gas adsorption, we still must answer the following questions: (1) Are our observations, made from an area a few hundred nanometers in extent, sufficiently representative to determine the mechanism for a specific reaction? (2) Is the reaction initiated by the incident electron beam? (3) Can we determine the sample temperature accurately enough to extract quantitative kinetic information? And (4), can we find efficient ways to make atomic-scale measurements from the thousands of images collected using a high-speed camera. The lack of global information available from TEM measurements is generally compensated by using other, ensemble measurement techniques such as x-ray or neutron diffraction, x-ray photoelectron spectroscopy, infrared spectroscopy, Raman spectroscopy etc. However, it is almost impossible to create identical experimental conditions in two separate instruments to make measurements that can be directly compared.

We have designed and built a unique platform that allows us to concurrently measure atomic-scale and micro-scale changes occurring in samples subjected to identical reactive environmental conditions by incorporating a Raman Spectrometer into the ESTEM. We have used this correlative microscopy platform i) to measure the temperature from a 60 µm$^2$ area using Raman shifts, ii) to investigate light/matter interactions in plasmonic particles iii) to act as a heating source, iii) to perform concurrent optical and electron spectroscopies such as cathodoluminescence, electron energy-loss spectroscopy and Raman. We have developed an automatic image-processing scheme to measure atomic positions, within 0.015 nm uncertainty, from high-resolution images, to follow dynamic structural changes using a combination of algorithms publicly available and developed at NIST. This method has been proven to capture the crystal structure fluctuations in a catalyst nanoparticle during growth of single-walled carbon nanotube (SWCNT). Details of the design, function, and capabilities of the optical spectrum collection platform and image processing scheme will be presented.

9:20am **NS+AS+EM+MI+SP+SS-ThM-5 Critical Dimension Metrology by Localization Optical Microscopy***, C Copeland, C McGray, J Geist, J Liddle, B Ilic, **Samuel Stavis,*** NIST

Optical microscopy methods of localizing subresolution emitters are broadly useful in many fields from biology to nanofabrication. Precision and accuracy are fundamental for localization measurements. Subnanometer precision is readily achievable for many emitters and can elucidate structure and motion at atomic scales, but is potentially false precision in the absence of calibrations that enable corresponding accuracy, particularly over a wide field for imaging and tracking. Whereas improving localization precision generally requires counting more photons by increasing emitter intensity and stability, improving localization accuracy presents diverse challenges in the calibration of an optical microscope as a measurement system. This involves not only its discrete components but also their interaction during a measurement. Such calibration is complex, motivating the development of practical devices and methods to facilitate the process, which we present here.

First, we characterize a complementary metal oxide semiconductor (CMOS) camera, enabling full use of its dynamic range and megapixel array. Next, we fabricate aperture arrays by electron-beam lithography and test them as calibration devices, exploiting their uniformity and stability. Then, we refine localization analysis, presenting a novel estimator and accommodating saturation. Finally, we evaluate aberrations of our optical system, including field curvature, distortion, and others that break the symmetry of the point spread function. After calibrating our system in this way, we validate our widefield measurements and demonstrate critical dimension localization microscopy (CDLM) of aperture arrays, and answer open questions about the apparent motion of nanoparticle fiducials. Our study casts new light on localization microscopy at subnanometer scales.

Our study also highlights the importance of nanoscale fabrication and metrology in achieving localization accuracy. Previous studies have applied aperture arrays for lens evaluation but have not quantified their critical dimensions, in particular the array pitch. This is essential to ensure that electron-optical aberrations do not propagate as errors through the calibration and correction of photon-optical aberrations. Moreover, the application of CDLM to aperture arrays provides useful information on the effects of dose delivery and beam scanning to optimize the future nanofabrication of reference materials.

9:40am **NS+AS+EM+MI+SP+SS-ThM-6 Tunable Emission from Nanophotonic Structures in a Modified SEM: Characterizing Smith Purcell Radiation Generation from the VUV to the Near IR***, **Steven Kooi,** I Kaminer, A Massuda, M Soljačić, C Roques-Carmes,* MIT

We present theoretical predictions and experimental results of multiple order Smith-Purcell radiation in a variety of samples from periodic high aspect ratio silicon nanowire structures to engineered metasurfaces using low-energy electrons (2.5 -20 keV) in a modified scanning electron microscope. The samples emit photons in a controlled way and we demonstrate optical emission from the VUV to the near IR, opening a pathway to building a fully tunable optical source that we intend to extend into the soft X-Ray regime.

11:00am **NS+AS+EM+MI+SP+SS-ThM-10 Ultrafast Optical Response of Graphene/LaAlO3/SrTiO3 Heterostructure***, L Chen, E Sutton, J Li, M Huang, J Hsu, B D'Urso,* University of Pittsburgh*; J Lee, H Lee, C Eom,* University of Wisconsin-Madison*; P Irvin, **Jeremy Levy,*** University of Pittsburgh **INVITED**

The unique electronic and optical properties of graphene make it a promising device in terahertz(THz) regime. Another 2D electron system, the complex-oxide heterostructure LaAlO3/SrTiO3, has been shown to exhibit great promise for control and detection of broadband THz emission at extreme nanoscale dimensions1. Recently, we have successfully integrated these two platforms: we have created graphene/LaAlO3/SrTiO3 structures with (1) high mobility in the graphene channel2 and (2) oxide nanostructures patterned directly underneath the graphene layer3. Here we describe new experiments that probe graphene with this nanoscale THz spectrometer using ultrafast optical techniques. This unprecedented control of THz radiation at 10 nm length scales creates a pathway toward hybrid THz functionality in graphene/LaAlO3/SrTiO3 heterostructures.

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11:40am **NS+AS+EM+MI+SP+SS-ThM-12 Single-Molecules Fluorescence Spectroscopy and Lifetime with Simultaneous Super-resolution Imaging for Materials Science Applications***, **James Marr,*** CNST/NIST and University of Maryland*; M Davanço,* CNST/NIST*; S Stranick,* NIST*; R Ilic, A Liddle,* CNST/NIST

We have developed a widefield imaging system that measures single-molecule position, orientation, lifetime and fluorescence spectra. We achieve this by combining conventional super-resolution imaging using an sCMOS detector with a unique, photon-counting, wide-field, high-temporal, high-spatial resolution, high-throughput, three-dimensional detector (H33D). The use of dual-objectives maximizes the fluorescent photon flux to each camera. Individual fluorophore point-spread functions collected by the sCMOS detector provide position and orientation information, while the 100 ps timing resolution of the H33D detector enables us to make precise lifetime measurements of the same fluorophore. By incorporating a diffraction grating into the beam path of the sCMOS camera we can simultaneously record both a zero-order image of each fluorophore for position and orientation measurement, and a wavelength-dispersed image that provides single-molecule spectroscopic data. The sensitivity of fluorophore lifetime, spectroscopic behavior, orientation, and position to dynamic processes in soft materials with nanosecond, millisecond, and second timescales, respectively, enables us to collect three-dimensional, local structure-property information that would otherwise be impossible to obtain. We have fabricated unique structures that enable us to accurately determine the influence of metallic and high-refractive index materials on fluorophore lifetime and point-spread function shape. Our far-field system, combined with these nanoengineered structures, permit minimally-perturbative measurements to be made on individual fluorophores. We apply our imaging system to probe the nanoscale behavior of polymers in nanocomposite materials and to investigate fluorophore response to structured samples consisting of thin, high-refractive index materials.

12:00pm **NS+AS+EM+MI+SP+SS-ThM-13 Atomic Scale Surface Effects of Controlled Crystal Structure in III-V Semiconductor Nanowires: Preferential Surface Alloying and Local Electronic Properties.***, J Knutsson, M Hjort,* Lund University, Sweden*; P Kratzer,* University Duisburg-Essen, Germany*; J Webb, S Lehmann, K Thelander,* Lund University, Sweden*; C Palmstrom,* UCSB*; R Timm, **Anders Mikkelsen,*** Lund University, Sweden

Despite the many III-V nanowire (NW) technologies under current development, be it solar cells and light emitting diodes or high speed/low power electronics, there are still only few studies of their surfaces. The atomic scale structure and morphology of NW surfaces are however central in determining their functionality, due to the inherently large surface to bulk ratio. In addition, III-V NWs can be tailored with segments of both the cubic zinc blende (ZB) and hexagonal wurtzite (WZ) structures and in a variety of materials combinations. This allow experimental access to nanocrystallite surfaces and interfaces not found in the bulk. We have demonstrated atomically resolved Scanning Tunneling Microscopy/Spectroscopy (STM/S) on a wide variety of these III-V NWs and on operational NW devices [1-5]. We now use these methods for studying atomic scale surface structural changes and impact on local electronic properties on both GaAs and InAs NWs at room temperature and at 5K.

We explore the surface diffusion and alloying of Sb into GaAs NWs with controlled axial stacking of Wz and Zb crystal phases. We find that Sb preferentially incorporates into the surface layer of the -terminated Zb segments rather than the -terminated Wz segments. Density functional theory calculations verify the higher surface incorporation rate into the Zb phase and find that it is related to differences in the energy barrier of the Sb-for-As exchange reaction on the two surfaces. These findings demonstrate a simple processing-free route to compositional engineering at the monolayer level along NWs.

Using low temperature STM/S we measure local density of states of atomic scale tailored Zb segments in Wz InAs nanowires down to the smallest possible crystal lattice change. We find that Zb crystal phase signatures can be seen in the density of states both on the conduction and valence band sides as well as in the band positions down to the smallest possible Zb segment. Additionally we find indications of confined state effects due to the difference in bandgap between Wz and Zb. Finally we explore the stability of InAs NWs with atomic scale STM during the application of voltages through the NWs in a device configuration. We observe that applying realistic voltages to InAs NWs results in removal of atomic scale defects and smoothening of the morphology.

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## Surface Science Division
## Room 25 - Session SS+EM+HC+MI-ThM

### Oxides: Structures and Reactions

**Moderators:** Valeria Lauter, Oak Ridge National Laboratory, Charles Sykes, Tufts University

8:00am **SS+EM+HC+MI-ThM-1 Influence of Iron Doping on Cobalt Oxide Bilayers on Au(111): Toward a Model of Synergistic Catalytic Effect in Oxygen Evolution Reaction***, **Jonathan Rodriguez-Fernandez**, Z Sun, J Fester, J Lauritsen,* Aarhus University, Denmark

Iron doped cobalt oxides have been shown enhanced activity for promoting the oxygen evolution reaction (OER) compared with unary iron oxides and cobalt oxides, respectively[1]. However, the nature of such synergistic catalytic effect and in particular the way of iron species incorporate with cobalt oxides are only understood on a superficial level, which presents a significant obstacle to further exploration on rational design of efficient OER catalysts. Noble metal supported transition metal oxides have been previously applied as model catalysts, which enables the powerful surface science techniques, and successfully reveal the catalytic active sites and help researchers understand the catalytic process further[2].

Here, aiming to study the origin of the synergistic catalytic effect, we dope iron into well-characterized cobalt oxide bilayer nanoislands supported on a single crystal Au(111) substrate[3]. Atomic-resolved scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS) are used to compare the growth of cobalt oxide and cobalt-iron oxide bilayers. We perform a comprehensive analysis of the iron doping induced influence on the atomic structure of the nanoislands and oxidation states of both the dopant and host species.

We find that doped iron species integrate into the cobalt oxide nanoislands and are mostly under oxidative condition. The Co atoms surrounding the doped Fe appear brighter and form 6-fold flower-like features under STM due to the local modification of electronic structure, which indicates changed chemical activities of these atoms. Similar situation happens on O atoms near doped Fe and form 3-fold triangle-like features. XPS spectra imply that Co keeps 2+ oxidation state whereas Fe shows 3+ oxidation state, which is not the same with the oxidation state of 2+ in the iron oxide nanoislands, indicating that iron species in the cobalt-iron oxides have stronger oxidizing ability. Further water exposure experiments demonstrate that hydroxyl groups usually appear next to the doped iron sites while almost randomly distributed on the basal plane of pure cobalt oxide nanoislands, suggesting that iron species in the cobalt-iron oxide play an important role in promoting the catalytic activity.

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8:20am **SS+EM+HC+MI-ThM-2 An Ordered Mixed Oxide Monolayer formed by Iron Segregation on Rutile-$TiO_2$(011)**, ***Sandamali Halpegamage,*** University of South Florida; *L Bignardi, P Lacovig,* Elettra-Sincrotrone Trieste, Italy; *A Kramer,* University of South Florida; *Z Wen, X Gong,* East China University of Science and Technology, PR China; *S Lizzit,* Elettra-Sincrotrone Trieste, Italy; *M Batzill,* University of South Florida

Ternary oxide monolayers supported on or intermixed with a second oxide surface have attracted great interest in designing new materials with unique chemical functional properties including selective heterogeneous catalysts and nanocatalysts. Due to the complexity of the structure and composition, it is challenging to discover and characterize such phases. Here we synthesized an ordered mixed oxide monolayer of $FeTi_2O_5$ on rutile-$TiO_2$(011) via two different experimental pathways; firstly, by annealing the clean $TiO_2$(011) in $1x10^{-7}$ mbar of $O_2$ at ~450 $^0$C and secondly, by physical vapor depositing Fe on clean $TiO_2$(011) in $1x10^{-7}$ mbar of $O_2$ at ~450 $^0$C.In both procedures the Fe atoms intermix with Ti atoms in the surface layer of the substrate and form an ordered mixed-oxide monolayer with $FeTi_2O_5$ composition. High resolution and fast X-ray photoemission spectroscopy (XPS) reveals that Fe and Ti are in 2+ and 4+ charge states respectively. The structure of this mixed oxide monolayer was predicted by a combination of atomically-resolved STM (Scanning Tunneling Microscopy) and DFT-based calculations and further confirmed by synchrotron based angle scanned x-ray photoelectron diffraction (XPD) studies. Multiple electron scattering simulations implemented in the Electron Diffraction in Atomic Clusters (EDAC) package were performed for comparing experimental XPD patterns with structural models. Judged by the reliability factor ($R_p$), the experimentally determined XPD patterns are in good agreement with the simulated XPD patterns. The study has been extended to a few of the other transition metals namely, V, Cr, and Ni. Due to the similarities in the bulk oxide structures of these transition metals they all are capable of forming similar intermixed monolayer oxide surfaces with the composition $MTi_2O_5$ (M=V,Ni,Cr). For all these monolayers, the valance band maximum (VBM) is above the VBM for $TiO_2$, suggesting that these monolayers may trap holes at the surface efficiently and thus may modify the photocatalytic activity of $TiO_2$.

8:40am **SS+EM+HC+MI-ThM-3 Growth and Chemistry of rutile $IrO_2$ Surfaces**, ***Jason Weaver***, *Z Liang, T Li, R Rai,* University of Florida, Gainesville; *M Kim, A Asthagiri,* The Ohio State University **INVITED**

Interest in the surface chemistry of late transition-metal oxides has been stimulated by observations that the formation of metal oxide layers tends to dramatically alter the catalytic performance of transition metals in applications of oxidation catalysis. In this talk, I will discuss our recent investigations of the growth and chemical properties of rutile $IrO_2$ surfaces. I will discuss our studies of the oxidation of metallic Ir surfaces by O-atom beams as well as $O_2$ at pressures above 1 Torr. We find that stoichiometrically-terminated $IrO_2$(110) layers could only be formed by oxidizing Ir(111) and Ir(100) at sufficiently high temperature and $O_2$ pressure. I will discuss the binding characteristics of small molecules, and our recent discovery of highly facile $CH_4$ activation on the $IrO_2$(110) surface at temperatures as low as 150 K.

9:20am **SS+EM+HC+MI-ThM-5 Formation and Manipulation of Water Clusters on Bilayer ZnO Surface**, ***Junseok Lee***, *D Sorescu, X Deng,* National Energy Technology Laboratory

Adsorption of water on the nanostructured metal oxide surfaces has implications in catalysis and serves as a prototypical system in studying water-oxide interfaces. By using scanning tunneling microscopy (STM) and density functional theory (DFT) calculations, the clustering behavior of water on the bilayer ZnO surface grown on Au(111) has been studied at low coverage regime. Diffusion and clustering of water molecules at specific sites in the Moire pattern are observed after initial adsorption of water on bilayer ZnO at T = 77 K. Heating the surface to T < ~240 K reveals that the adsorbed water molecules form triangular shape clusters with two specific orientations in the STM images. The DFT calculations along with the experimental findings suggest that the clusters are comprised of mixed water and hydroxyl groups with a binding energy of 21 kcal/mol. The two types of clusters can be converted to each other by the injection of electron from the STM tip. The inelastic electron scattering process is considered to be responsible for the conversion of the clusters via O-H stretch vibration mode excitation.

9:40am **SS+EM+HC+MI-ThM-6 Formation of Metastable Water Chains on Anatase $TiO_2$(101)**, ***Arjun Dahal***, *Z Dohnálek,* Pacific Northwest National Laboratory

The interaction of water with metal oxide surfaces is of great importance in many diverse areas such as catalysis, electrochemistry, corrosion, atmospheric science, geology, astrophysics, and others. Anatase $TiO_2$ surface is particularly relevant because it is the most active polymorph of $TiO_2$ and its commercially employed nanomaterials grow preferentially as anatase. In this study, we employ scanning tunneling microscopy (STM) to study the adsorption of water on a model stoichiometric anatase $TiO_2$(101) surface. Well-defined anatase $TiO_2$(101) surface has saw-tooth-like morphology exposing alternating rows of two-fold-coordinated oxygen atoms ($O_{2c}$) and five-fold-coordinated Ti atoms ($Ti_{5c}$) along the [010] direction. Our STM data show that at 80 K isolated water monomers bind molecularly to the $Ti_{5c}$ sites. The onset of diffusion is found at ~190 K where water monomers diffuse both along and across the $Ti_{5c}$ rows. The analysis shows that the along-the-row diffusion is energetically favored by only 0.03 eV. Surprisingly, we find that at 80 K water molecules start to form linear chains along the $Ti_{5c}$ rows as the coverage is increased. This indicates the presence of transient mobility of water molecules suggesting that the adsorption occurs via a precursor state. When the water chains are annealed at 190 K, they fall apart to monomers that reside on the next-nearest-neighbor $Ti_{5c}$ sites. These results demonstrate that the water chains are metastable in nature. This is at odds with many other oxide surfaces where hydrogen-bonded water clusters are energetically preferred over the isolated monomers.

11:00am **SS+EM+HC+MI-ThM-10 The Structure of $Fe_2O_3$(012) and its Reactivity to Water**, ***Gareth Parkinson***, *F Kraushofer, Z Jakub, M Bichler, J Hulva, M Schmid, U Diebold, P Blaha,* TU Wien, Austria

Hematite ($\alpha$-$Fe_2O_3$) is a promising material for technological applications due to its abundance, low cost and chemical stability. Its 2.2 eV bandgap makes it potentially ideal as a photoanode for photoelectrochemical water splitting, [1] but performance is hampered by slow reaction kinetics and the need for a significant overpotential. Little is known about the atomic-scale structure of hematite surfaces, and even less about how this relates to photocatalytic activity.

To date, most surface science studies of $\alpha$-$Fe_2O_3$ have focused on the (001) facet, but preparing a stoichiometric surface under UHV conditions has proven problematic. Some authors have investigated the equally relevant (012) surface, [2][3][4] and reported that a (1x1) and a reduced (2x1) termination can be reversibly prepared. Several models have been proposed for the (2x1) reconstruction, but as yet no scanning probe data exists to support or refute them.

Here we present a multi-technique study of the (1x1) and (2x1) surfaces of $\alpha$-$Fe_2O_3$ (012), as well as their interaction with water. The data acquired for the (1x1) termination support a bulk termination model, as predicted by previous publications, but STM and nc-AFM images of the (2x1) reconstruction are inconsistent with previously proposed models. [3] We propose a new model based on ordered oxygen vacancies, the plausibility of which is confirmed by density functional theory (DFT) results. TPD and XPS data reveal that the (1x1) surface adsorbs water in a mixed-mode fashion, whereas the interaction with the (2x1) surface is entirely dissociative. We propose models for the structure of the adsorbed overlayers based on scanning probe microscopy data.

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11:20am **SS+EM+HC+MI-ThM-11 Interaction of Water with anatase $TiO_2$(001)-1x4**, ***Igor Beinik***, *K Adamsen, S Koust, J Lauritsen, S Wendt,* Aarhus University, Denmark

The interaction of water with titanium dioxide ($TiO_2$) is pivotal for many practical applications of this material in heterogeneous catalysis because water is almost always present either as a reactant or a product in many catalytic reactions. In our model study, we focus on the anatase polymorph of $TiO_2$ that has demonstrated a higher catalytic activity in water splitting than rutile and is generally considered as a more technologically relevant polymorph. The nanocrystals of anatase that are present in powder catalysts normally expose a high fraction of low surface energy (101) facets and a significantly smaller fraction of high energy, but supposedly more reactive (001) facets. The (001) facet is intrinsically unstable and reconstructs upon annealing in vacuum forming 1x4 reconstructed terraces, where rows of bridging oxygen atoms in [100] and [010] directions are replaced by $TiO_3$ units [1]. This kind of reconstruction has been found both on the (001) facets of anatase single crystals and nanoparticles [2], however the interaction of water with this surface has been significantly less investigated.

In the present work, we study the adsorption and dissociation of water on the anatase (001) 1x4 reconstructed surface by means of STM, TPD, and synchrotron core-level and valence band PES under UHV conditions. Our results show that water dissociates to some extent even at 120 K and that low water exposures (up to 3 L) at this temperature results in a mixture of molecularly and dissociatively adsorbed molecules. A systematic analysis of the data obtained using all three techniques leads us to a conclusion that the A-TiO2(001)-1x4 surface is rather reactive - in agreement with an earlier study [3] we find that water dissociates at the ridges of the 1x4 reconstruction. Moreover, the 1x4 reconstruction remains stable upon water exposures at least up to ~45 L (at 120 K). However, after desorption of a multilayer ice film, the ridges themselves contain a high number of defects, which remain stable up to 800 K. The nature of these defects will be discussed.

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## Electronic Materials and Photonics Division
## Room 14 - Session EM+NS-ThA

### Wide and Ultra-wide Band Gap Materials for Electronic Devices: Growth, Modeling, and Properties

**Moderators:** Michael Filler, Georgia Institute of Technology, Rachael Myers-Ward, U.S. Naval Research Laboratory

2:20pm **EM+NS-ThA-1 Synthesis of β-Ga2O3 Thin Films on SiC by Molecular Beam Epitaxy***, **Neeraj Nepal**, D Katzer, D Storm, M Hardy, B Downey, D Meyer,* U.S. Naval Research Laboratory

Recently, there has been great interest in β-Ga2O3 as a next generation ultra-wide bandgap semiconductor (UWBGS) for high-power/temperature electronics devices. However, it has low thermal conductivity of β-Ga2O3 may limit device performance. One strategy to improve performance of Ga2O3 based devices is through heterostructure design on high thermal conductivity substrate. In this paper, we report growth and characterization of 100 nm thick β-Ga2O3 on SiC by molecular beam epitaxy (MBE) at 650 °C. First, the growth parameter space such thermocouple measured growth temperature, relative Ga flux, and oxygen plasma were varied to grow β-Ga2O3 films on c-plane sapphire substrates. For an O2 plasma flow of 1 sccm (2.5x10-5 torr) X-ray diffraction shows weak facets of β-Ga2O3 appear regardless of the Ga flux and temperature, however for <0.6 sccm O2 flow, smooth β-Ga2O3 [ (-201)||(0001)] grows on c-plane sapphire. Optimized MBE growth conditions on sapphire substrate were used to grow β-Ga2O3 on SiC. Single phase MBE β-Ga2O3 film on SiC grown at 650 °C are insulating, have rocking curve full-width-at-half-maximum of 720 arc-sec with root mean square surface roughness of less than 2 nm. In this paper we will discuss MBE growth parameter space of β-Ga2O3 on sapphire and the structural, morphological, and electrical properties of MBE grown β-Ga2O3 thin films on SiC.

2:40pm **EM+NS-ThA-2 Growth and Characterization of *α*-, *β*-, and *ε*-$Ga_2O_3$ Epitaxial Layers***, **Lisa Porter**, Y Yao, L Lyle,* Carnegie Mellon University*; S Okur, G Tompa, T Salagaj, N Sbrockey,* Structured Materials Industries, Inc.

Increasing global demand for energy makes urgent the need for highly efficient high-power electronics for energy conversion and transport. Although silicon devices have been traditionally used for high-power electronics, wide bandgap semiconductors (e.g., SiC and GaN) are much more efficient for these applications, because they can withstand higher electric fields with less material and reduced energy loss. However, the substrates of both materials are still very expensive. A very promising alternative to SiC and GaN is gallium oxide, $Ga_2O_3$, which has an even larger bandgap than the former two materials. The availability of this material presents new possibilities for disruptive devices and technologies that could translate to even greater energy efficiencies at lower cost than predicted for SiC and GaN. Polished 2-in diameter, single-crystal wafers of the monoclinic *β*-phase can be grown using melt-growth methods and are commercially available. However, there is increasing interest in the other $Ga_2O_3$ phases, particularly the metastable corundum-structured *α*- and hexagonal-structured *ε*-$Ga_2O_3$ phases because of their higher symmetry and simpler epitaxial relations to c-plane sapphire, in addition to the possibility of producing functional heterostructures or tunable bandgaps through alloying. We have successfully grown epitaxial films of *α*-, *β*- and *ε*-phases on c-plane sapphire using different precursors and growth conditions. The *α*- and *ε*-phases have generally been reported in the literature to form at lower growth temperatures than the *β*-phase. However, we observed a change in phase formation at the same growth temperature by changing our growth technique and Ga precursor from metalorganic chemical vapor deposition (MOCVD) and trimethlygallium to halide vapor phase epitaxy (HVPE) and gallium chloride. Data from x-ray diffraction, scanning electron microscopy and high-resolution transmission electron microscopy will be presented to illustrate the different epitaxial films and orientation relationships. The results of secondary ion mass spectrometry depth profiles, which showed compositional differences within the different phases, will also be presented. The authors wish to acknowledge the Office of Naval Research under contract no. N00014-16-P2059.

3:00pm **EM+NS-ThA-3 Ultra-wide-bandgap $Ga_2O_3$ Material and Electronic Device Technologies***, **Masataka Higashiwaki**, M Wong,* National Institute of Information and Communications Technology, Japan*; K Konishi,* Tokyo University of Agriculture and Technology, Japan*; Y Nakata, T Kamimura,* National Institute of Information and Communications Technology, Japan*; K Sasaki, K Goto,* Tamura Corporation, Japan*; A Takeyama, T Makino, T Ohshima,* National Institutes for Quantum and Radiological Science and Technology, Japan*; H Murakami, Y Kumagai,* Tokyo University of Agriculture and Technology, Japan*; A Kuramata, S Yamakoshi,* Tamura Corporation, Japan **INVITED**

Recently, gallium oxide ($Ga_2O_3$) has attracted much attention as a candidate for future power and harsh environment electronics due to its extremely large bandgap of 4.5 eV and the availability of economical melt-grown native substrates. In this talk, following a short introduction of the material properties of $Ga_2O_3$, we will discuss our recent progress in the development of $Ga_2O_3$ metal-oxide-semiconductor field-effect transistors (MOSFETs) and Schottky barrier diodes (SBDs), including $Ga_2O_3$ thin-film epitaxial growth technologies by molecular beam epitaxy (MBE) and halide vapor phase epitaxy (HVPE).

State-of-the-art $Ga_2O_3$ MOSFETs with a gate-connected field plate (FP) were fabricated using MBE-grown $Ga_2O_3$ homoepitaxial layers. The devices showed excellent room-temperature (RT) characteristics such as a record high off-state breakdown voltage ($V_{br}$) of 755 V, a large drain current on/off ratio of over nine orders of magnitude, and DC-RF dispersion-free output characteristics [1]. Furthermore, the MOSFETs demonstrated strong prospects of $Ga_2O_3$ devices for extreme environment electronics by virtue of their stable high-temperature operation up to 300°C and strong radiation hardness against gamma-ray irradiation [2].

We have also fabricated and characterized $Ga_2O_3$ FP-SBDs on $n^-$-$Ga_2O_3$ drift layers grown by HVPE [3-5]. The illustrative device with a net donor concentration of $1.8\times10^{16}$ cm$^{-3}$ exhibited a specific on-resistance of 5.1 mΩ·cm$^2$ and an ideality factor of 1.05 at RT. Successful FP engineering resulted in a high $V_{br}$ of 1076 V. Note that this was the first demonstration of $V_{br}$ of over 1 kV in any $Ga_2O_3$ power device. The maximum electric field in the $Ga_2O_3$ drift layer at the condition of destructive breakdown was estimated to be 5.1 MV/cm by device simulation, which is about two times larger than the theoretical limits for SiC and GaN.

This work was partially supported by Council for Science, Technology and Innovation (CSTI), Cross-ministerial Strategic Innovation Promotion Program (SIP), "Next-generation power electronics" (funding agency: NEDO).

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4:00pm **EM+NS-ThA-6 Reactive Magnetron Sputtering of Titanium Nitride and Titanium Aluminum Nitride on Lithium Niobate for Electronic and Opto-Electronic Applications***, **Amber Reed**, H Smith, D Abeysinghe, P Shah, L Grazulis, M Hill, M McConney, B Howe, A Urbas,* Air Force Research Laboratory

High temperature stability, hardness, abrasion resistance, chemical stability and potential complimentary metal-oxide semiconductor process compatibility, combined with a high electrical conductivity make titanium nitride (TiN) an important material for electronic and opto-electronic applications. TiN is particularly important as an electrode material due to its oxidation resistance, which can be improved by alloying it with aluminum nitride to form titanium aluminum nitride ($Ti_{1-x}Al_xN$). In addition to its use as an electrode, TiN is also a promising plasmonic material because, similar gold, it possesses a zero crossover wavelength in the visible region. The ability to synthesize high quality TiN crystals on different electronic substrates would greatly facilitate its incorporation in electronic and opto-electronic devices. One particular material of interest is lithium niobate ($LiNbO_3$), which possesses unique piezoelectric, opto-electronic and nonlinear optical properties. Synthesis of high quality TiN on $LiNbO_3$ would allow for integration of TiN into acoustic devices (i.e. SAWs and BAWs), optical modulators, and other electronic and opto-electronic devices.

In this work, we demonstrate the synthesis of high quality epitaxial TiN crystals on Z-cut $LiNbO_3$ substrates. We also discuss the growth of TiN and $Ti_{1-x}Al_xN$ on Y-cut $LiNbO_3$. While the (001) plane of Z-cut $LiNbO_3$ creates a template for epitaxial growth of (111)-oriented TiN crystals, similar to growth on (001)-oriented sapphire, the (010) plane of Y-cut $LiNbO_3$ is equally lattice matched to the TiN (001) and (101) planes which results in competitive growth of those two orientations. Alloying the TiN with AlN exacerbates this issue as the lattice constant shrinks with increased AlN content. We investigate the role of deposition power, nitrogen gas fraction, and substrate temperature and ion flux impingement on the competitive growth to determine the optimal growth conditions to promote epitaxy. Films are characterized using x-ray diffraction (XRD), atomic force microscopy (AFM), transmission electron microscopy, ellipsometry and electrical measurements. XRD and AFM of TiN on Z-cut $LiNbO_3$ show remarkably smooth (< 220 pm RMS roughness) epitaxial films. Ellipsometry measurements of the TiN on Z-cut $LiNbO_3$ reveal carrier concentrations up to 4.0 $x10^{22}$ $cm^{-3}$, mobilities of ~3.2 $cm^2/(V\ s)$ and a $\varepsilon_1/\ \varepsilon_2$ of 1.00 to 3.34 at a wavelength of 1550 nm.

4:20pm **EM+NS-ThA-7 Growth and Property Analysis of Doped GaN-GaAlN Heterostructures on Low- and High-temperature AlN/Sapphire Templates***, **Nikolaus Dietz**, B Cross, M Vernon,* Georgia State University*; R Collazo, R Kirste, S Mita, Z Sitar,* North Carolina State University

The developing of radiation-hard UV solid state avalanche photodiodes (APD's) based on group III-Nitride wide band gap materials have a wide application area from solar blind detector to wavelength specific PMT based detector devices that can be tuned in the 220 nm to 450 nm wavelength range, tailored to specific scintillators of interest. This contribution focuses on closely lattice-matched, high-quality GaN a substrate technologies using metalorganic chemical vapor deposition (MOCVD) technique, which provide sufficient high-quality AlGaN layers and heterostructures with high phase uniformity and low dislocation density for low leakage currents, to enable avalanche mechanisms, low leakage currents, high performance characteristics and reliability of the devices.

We will present results on the growth and doping of GaN/GaAlN heterostructures deposited on low- and high-temperature AlN/Sapphire template structures, using a customized D125 Veeco MOCVD reactor system. The structural quality of the initial GaN layer grown on various AlN-/GaN-sapphire template structure has been analyzed and is accessed regarding its resulting dislocation and defect densities, using XRD, Raman and FTIR spectroscopy. The influence of Silicon n-doping in GaN and $Ga_{0.9}Al_{0.1}N$ epilayers on the defect density was analyzed XRD and the dopant incorporation by SIMS analysis.

4:40pm **EM+NS-ThA-8 A Thermodynamic Supersaturation model for the Growth of AlGaN by MOCVD***, **Ramón Collazo**, S Washiyama, I Bryan,* North Carolina State University*; P Reddy, S Mita,* Adroit Materials Inc.*; Z Sitar,* North Carolina State University **INVITED**

AlGaN have been considered to be essential for the development of optoelectronic and electronic devices such as deep UV LEDs and other power devices. However, even under well-controlled growth conditions it is difficult to precisely predict the behavior of AlGaN growth with regards to Al-concentration and related defect incorporation. We have developed a thermodynamic model for the calculation of the Ga supersaturation during the growth of GaN by metalorganic chemical vapor deposition (MOCVD), which was successfully used to predict incorporation of impurities such as carbon as well as the surface morphology (Mita et al., JAP 104, 13521). This model was extended to evaluate the supersaturation of Al and Ga in AlGaN growth and to allow for the prediction of the properties of MOCVD grown AlGaN layers. Non-linear equations for Al and Ga equilibrium vapor pressure calculation describe the process under the following assumptions: (1) under low total pressure, gas phase reactions between the metalorganics and $NH_3$ are negligible; the III metal precursors are irreversibly cracked on the growth surface, thus, Al, Ga, $NH_3$, $H_2$ and $N_2$ are analyzed; (2) number of moles of growing species are conserved; (3) at least some $NH_3$ molecules are thermally cracked in the gas phase. Using the resulting model, the influence of growth parameters such as V/III and flow rate on AlGaN growth was determined through the dependence of the Ga and Al supersaturation. The independent parameters for the calculations included the growth conditions that were set by typical conditions for AlGaN MOCVD growth. Calculation showed a significantly lower equilibrium vapor pressure for Al ($10^{-12}$-$10^{-16}$ Torr) than for Ga ($10^{-4}$-$10^{-6}$ Torr). The Ga equilibrium pressure monotonously decreased with increasing V/III ratio, while $NH_3$ thermal cracking was more significant on the equilibrium pressure, as expected from Le Chatelier`s principle. The significant difference in the supersaturation between Ga and Al has a significant influence on the growth of ternary AlGaN compounds and need to be considered for finding appropriate and robust growth conditions at high temperatures, exceeding 1150 ºC. A processing AlGaN compositional phase diagram dependent on the typical growth conditions will be presented. In addition, experimental validation of this model with respect to Al composition, process stability and robustness will be discussed. This validation will be presented in terms of temperature and V/III ratio.

5:20pm **EM+NS-ThA-10 Anomalous Hall Effect in MOCVD-grown Gadolinium-doped Gallium Nitride***, V Saravade, P Patel, C Ferguson, K Yunghans, A Ghods, C Zhou, **Ian Ferguson**,* Missouri University of Science and Technology

Dilute Magnetic Semiconductor (DMS) materials for spintronics applications have the potential to reduce power consumption while increasing the processing speed, integration densities and non-volatile memory, compared to the conventional semiconductor devices. While Gd-doped GaN has exhibited room temperature (RT) ferromagnetism, the Anomalous Hall Effect (AHE) has not been reported in relation to the observed magnetic properties [1, 2].

In this work, we study the AHE in MOCVD-grown Gd-doped GaN with different Gd concentrations and precursors, and investigate their magnetic properties. RT AHE along with XRD helps in determining the mechanisms responsible for the observed ferromagnetism. Our preliminary measurements showed residual $R_{xy}/R_{xx}$ up to 10 and residual coercive field up to 50 Oe. These hysteresis curves can be caused by the ferromagnetic properties of MOCVD-grown Gd-doped GaN. Additionally, GaN (002) peak had been identified in the initial $\Omega$-2$\theta$ XRD scans. XRD rocking curve scans with varying $\Omega$ will be performed to study, the defects that are induced by doping GaN with Gd, and their potential contribution towards ferromagnetism. AHE and XRD results of Gd-doped GaN will be compared to those of un-doped GaN to verify that the ferromagnetism is caused by Gd doping. Furthermore, the effect of temperature on the magnetic behavior of Gd-doped GaN will be analyzed using variable temperature AHE.

To our knowledge, we are the first to report the AHE in MOCVD-grown Gd-doped GaN. We consider this work to contribute towards the investigation of DMS for RT ferromagnetism and further for spintronics applications.

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5:40pm **EM+NS-ThA-11 Valence and Conduction Band Offsets of $Al_2O_3$, $LaAl_2O_3$, AZO and ITO with $Ga_2O$-$_3$***, **Patrick Carey IV**, F Ren, D Hays, B Gila, S Pearton,* University of Florida*; S Jang,* Dankook University, South Korea*; A Kuramata,* Tamura Corporation, Japan

Band alignments for $Al_2O_3$, $LaAl_2O_3$ (LAO), Aluminum Zinc Oxide (AZO), and Indium Tin Oxide (ITO) with bulk β-$Ga_2O_3$ were determined by X-ray Photoelectron Spectroscopy. β-$Ga_2O_3$ is a direct band gap, ~4.9 eV, semiconductor, it has a very high theoretical breakdown electric field (~8 MV/cm), and is suitable for high power electronics in industrial, military applications, deep-UV photodetectors for a cut-off wavelength of 280 nm, and high temperature gas sensors. Ohmic contact with low contact resistance and gate oxides with low leakage current are essential for fabricating high performance base $Ga_2O_3$ electronic and optical devices. Since $Ga_2O_3$ has a wide energy bandgap, it is difficult to form low resistance Ohmic contact with conventional metal contact. ITO and AZO were found to have a conduction band offset of gap of -0.32 and -0.79 eV, respectively, which can be used as an intermediate layers between the metal contact and $Ga_2O_3$ to reduce contact resistance on $Ga_2O_3$-based devices. For wider energy band oxides, for use as gate oxides, sputtered LAO, atomic layer deposited (ALD) and rf-magnetron sputtered $Al_2O_3$ were employed. LAO was found to have a bandgap of 6.5 eV, a valence band offset of -0.21 eV, and a conduction band offset of 2.01 eV. LAO has a type II alignment and would provide excellent electron confinement, but no barrier for hole transport. $Al_2O_3$ was found to have a bandgap of 6.9 eV regardless of preparation method. However, the deposition method affected the band alignment. For ALD $Al_2O_3$, it has a has a nested (type I) gap alignment with a valence band offset of 0.07eV and a conduction band offset of 2.23 eV. While for sputtered $Al_2O_3$ on the same $Ga_2O_3$, there is a type II alignment with a valence band offset of -0.86 eV and a conduction band offset of 3.16 eV. The conduction band offsets in either case are large and provide excellent electron confinement, but the valence band offsets are smaller than desirable for limiting hole transport.

6:00pm **EM+NS-ThA-12 *In Situ* Plasma Emission Spectroscopy of InN/GaN Heterostructures Grown by MEPA-MOCVD*, Daniel Seidlitz,*** *B Cross, Y Abate,* Georgia State University*; A Hoffmann,* Technical University of Berlin, Germany*; N Dietz,* Georgia State University

In this study, we will present results of the in-situ plasma emission spectroscopy (PES) of the plasma activated nitrogen species during the growth of GaN/InN heterostructures by MEPA-MOCVD in correlation to their optical and structural characteristics.

Indium-rich InGaN semiconductors are of high interest due to the high electron mobility which enables ultrafast electronics operating in the THz regime. In conventional MOCVD, indium incorporation above 25 % is a challenge due to the vastly different partial pressures between InN and GaN and the lattice mismatch between the binaries. Migration enhanced plasma-assisted MOCVD is a kinetic stabilized growth surface approach to reduce the partial pressure difference between the InN and GaN. It also replaces the traditional ammonia precursor source for nitrogen through energetically controlled ionized nitrogen species (N*/NH*/NHx*), generated by a radio-frequency hollow cathode (13.56 MHz) with an output power between 50-600 W. The plasma-excited species are tailored in the gas phase and directed to the growth surface in the afterglow regime of the remote plasma utilizing the kinetic energies of the active nitrogen species to achieve a stable growth surface. Altering the process parameters like reactor pressure and nitrogen flux allows variation of the kinetic energies. A grid between the plasma source and the growth surface enables the control of the charged species reaching the growth surface and with it the electrostatic interactions in the InN/GaN growth process and the resulting layer properties. In-situ real-time plasma emission spectroscopy (PES) is used to monitor and identify the active nitrogen species close to the hollow cathode as well as near the growth surface. Comparison of the spectra could help to determine which nitrogen species promote the growth of group III- nitride materials.

Optoelectronic and structural qualities such as free carrier concentration as well as crystallinity, growth rate, the surface morphology of the GaN and InGaN films are examined using ex-situ characterization techniques (Raman, AFM, FTIR). We will present a correlation of the in-situ and ex-situ results as a function of the explored growth parameters like growth temperature, plasma power, and reactor pressure.

## Surface Science Division
## Room 25 - Session SS+AS+EM-ThA
## Semiconductor Surfaces

**Moderators:** James Ohlhausen, Sandia National Laboratories, Petra Reinke, University of Virginia

2:20pm **SS+AS+EM-ThA-1 Visualizing the Nanoscale Electrostatics of Material Interfaces*, Vincent LaBella,*** SUNY Polytechnic Institute*; W Nolting,* University at Albany, SUNY **INVITED**

Electrostatic barriers at material interfaces are the foundation of electronic and optoelectronic devices. Their nanoscale uniformity is of paramount concern with the continued scaling of devices into the sub 10 nm length scale and the development of futuristic nanoscale devices. This creates a fundamental and technological need for nanoscale insight into the fluctuations of electrostatic barriers at material interfaces. This presentation will focus on our development of visualizing the nanoscale electrostatic fluctuations that are occurring at metal-semiconductor and metal-insulator-semiconductor interfaces. This is accomplished by acquiring tens of thousands of ballistic electron emission microscopy spectra on a grid and fitting them to get the local Schottky barrier height. Both false color images as well as histograms of barrier heights are then created and compared to theoretical modeling. This has given new insight into both the scattering of the hot electrons and the interface composition and their effect on the electrostatics. For example, interfaces with incomplete silicide formation and mixed metal-species interfaces have been imaged and when combined with cross-sectional TEM provide new insight into their effects on the electrostatics that is not possible with conventional bulk transport measurements or other metrology techniques.

3:20pm **SS+AS+EM-ThA-4 Reactions of Benzoquinone with Hydrogen Terminated Silicon Surfaces*, Meixi Chen,*** *J Hack, A Iyer, R Opila,* University of Delaware

Iodine and Quinhydrone(QHY) dissolved in methanol have long been known to react with hydrogen terminated silicon surfaces to passivate electronic defects where photo-excited carriers recombine non-radiatively. The mechanism of this passivation is not well understood. The two constituent parts p-benzoquinone(BQ) and hydroquinone(HQ) have been studied separately in this work. We have shown that even though BQ and HQ are a redox couple, they behave very differently in reacting with silicon surfaces. The reaction is photolysis, pH sensitive and solvent-dependent. X-ray photoelectron spectroscopy (XPS) and cyclic voltammetry were used to show that the BQ reacted with the surface. The electrical passivation of silicon surfaces is confirmed by carrier lifetime measurements where the silicon surface recombination velocity is deceased to 11cm/s. Changes in surface band bending are observed in XPS surface photovoltage. DFT calculations have also been performed. The reaction mechanism will be discussed in detail.

4:00pm **SS+AS+EM-ThA-6 Uniform Reactivity and Bonding between Si(100) and GaAs(100) Wafers using Low Temperature (<180°C) Wet NanoBonding™ Optimized by Surface Energy Analysis*, Nicole Herbots,*** *R Islam,* Cactus Materials

Bonding two semiconductors surfaces such as Si and GaAs can increase performance in solar cell efficiency and high power electronics. In this work, the surface chemistry and topography of Si and GaAs are investigated to optimize the bonding of the pair. A new process called Nano-bonding™ [1,2 ] can nucleate cross-bonding molecules via electron exchange between two surfaces into a macroscopically continuous bonding "inter-phase" . The surfaces to be bonded are first chemically smoothed at the nano-scale and then terminated with matching "precursor phases". When activated, these phases exchange electrons. In other words, one surface is prepared so that it interacts preferentially with electron acceptors while the other surface is prepared to preferentially interact with electron donors. Hence, the precursor phases must be stable in air at room temperature until the surfaces are put into contact in clean-room class 10/ISO2 conditions and at low temperature (< 180°C). To bring the two surfaces into uniform contact while activating electron exchange and cross-bonding reactions, isotropic steam pressurization is applied, hence the name "Wet" Nano-Bonding™ [1,2].

The precursor phases are optimized based on insights provided by the Van Oss theory, combined with characterization of composition via Ion Beam Analysis (IBA), with surface energies via Three Liquids Contact Angle Analysis (3LCAA) and with surface topography using Atomic force Microscopy. On smooth surfaces, the Van-Oss theory separates contributions to the total surface energy $\gamma^T$ into molecular interactions $\gamma^{LW}$, and interactions with electrons donors $\gamma^+$ and acceptors $\gamma^-$. These can then be each extracted accurately from 3LCAA measurements [2] using multiple (>3) drops. NanoBonding™ is observed when surface pairs complement each other for electron exchange: one surface with high $\gamma^+$ and the other with high $\gamma^-$ leads to the formation of molecular cross-bonds. However, IBA and 3LCAA characterization results show that this criteria is not sufficient. The total surface energies $\gamma^T$ for both GaAs, and Si must be larger than 40 mJ/m$^2$. This is due to the fact that the contribution of interactions with electron donors and acceptors needs to amount to at least 10-15% of $\gamma^T$, so that total surface interaction $\gamma^T$ is not mostly controlled by molecular interactions $\gamma^{LW}$ , but exhibits significant non-molecular interactions with both acceptors and donors. Only then can the dominance of interactions with acceptors on one surface and interaction with donors on the other surface promote NanoBonding™ effectively.

[1] Herbots N. et al. US Patent 9,018,077 (2015); 9,589,801 (2017).

4:20pm **SS+AS+EM-ThA-7 Evaluation of Silicon Oxidation in Downstream Plasma Photoresist Strip with Reducing Chemistries*, Tongchuan Gao,*** *V Vaniapura,* Mattson Technology, Inc.

With the rapid development of ultra-shallow junction depth devices, minimized silicon surface damage with the photoresist (PR) strip processes is stringently required. Silicon oxidation associated with the strip processes results in silicon loss, and, therefore, adversely affects the source-to-drain current of the devices. This leads to an ongoing effort to develop strip processes with both high PR ash rate and low silicon oxidation rate. The commonly used PR removal technique, downstream oxidizing chemistry plasma, may result in significant silicon surface oxidation. Recently, reducing chemistry has been extensively investigated for PR stripping with very low silicon surface damage.

To understand the silicon oxidation behavior with PR removal using reducing chemistries, a series of experiments were conducted. Silicon wafers with controlled pre-processing native oxide thickness were treated in an inductively coupled plasma downstream reactor with different reducing chemistries. Processes with different reducing chemistry composition, plasma source power, processing time, and post-processing queuing time were systematically studied. Comparison was also made between reducing and oxidizing chemistries. The oxide growth was reduced by tuning the reducing chemistries as well as the hardware configuration. Ellipsometry and X-ray photoelectron spectroscopy (XPS) were used for oxide thickness measurement and quantitative chemical composition analysis for the pre- and post-processing wafers, respectively.

The experimental results demonstrated that higher $H_2$ content in the chemistry leads to more oxide growth, which may be attributed to that energized hydrogen species break the Si-Si bonds and then oxidation takes place, or that hydrogen can penetrate the silicon substrate and then are replaced by oxygen. Time-dependent oxidation tests showed that the oxide growth rate is higher for silicon wafers with thinner pre-processing native oxide layer due to the self-limiting nature of oxide growth. Most of the oxide growth happens within the first 30 seconds of the processes. PR ash rate and uniformity were monitored correspondingly to ensure satisfactory PR removal. Our work sheds light on the optimization of reducing chemistry plasma processes for efficient PR removal with minimal silicon oxidation.

4:40pm **SS+AS+EM-ThA-8 Surface-sensitive Measurement of Dielectric Screening via Atom and Electron Manipulations**, ***Daejin Eom**, E Seo, J Koo,* Korea Research Institute of Standards and Science, Republic of Korea

Dielectric screening is essential in determining semiconductor properties. Its assessment on the surface, however, is beyond the capability of conventional capacitance and optical techniques due to their lack of surface sensitivity. Here we present the surface-sensitive measurement of the dielectric screening by using the scanning tunneling microscopy and spectroscopy. To be specific, we generate a single-atom defect on the surface and vary its ionization state by a single-electron charge. We then assess in-plane dielectric constant and Debye length at the surface by probing the surface potential modulation with atomic resolutions. Such single-atom and single-electron manipulations on B δ-doped Si(111) surface unravel that the dielectric screening on this surface is much in excess of what the classical image-charge model predicts, which we ascribe to the strained bonds and the ionic character of the surface layers. Also, as an exemplary application of the measured screening parameters, we demonstrate determining the ionization state of a surface defect from the defect-induced band bending.

5:00pm **SS+AS+EM-ThA-9 The Effects of UV Irradiation, Stage Temperature, and Radical Flux on UV-Ozone Treatment using High-aspect-Ratio Cave Structures**, ***Shogo Uehara**, T Sugawara, P Wood,* SAMCO Inc.

UV-ozone treatment provides an atomic oxygen chemical reaction, where oxygen radicals are produced by UV-induced or thermal dissociation of ozone. Previously, it was found that ozone flux and stage temperature were critical for wettability improvement of polymer substrates such as polyetheretherketone (PEEK) [1]. However, in that study, the effects of UV irradiation, temperature, and oxygen radical flux were not clearly distinguished. In this research, a cave structure was employed to better elucidate the reaction mechanisms of UV irradiation, substrate temperature, and radical flux in UV-ozone treatment.

Polyimide-coated and photoresist-coated silicon coupons (5 mm x 5 mm) were placed at various depths inside a straight aluminum cave (6 mm x 6 mm square and 96 mm maximum depth). A SAMCO model UV-2 was used for this study. This system employs a cold cathode, mercury vapor UV lamp (185 nm and 254 nm), a remote (ex-situ) silent discharge high-concentration ozone generator (30-160 $g/m^3$) and sample stage heating (50 to 200°C). The surface wettability of polyimide was examined using the water contact angle, and the photoresist ashing rate was measured using a stylus profilometer (Ambios Technology, XP-200).

Generally, samples placed at higher aspect ratios showed higher contact angles and lower ashing rates. This indicated that the reactive species were deactivated or did not reach the sample when the aspect ratio became larger (i.e. the depth of the sample in the cave became greater). At an aspect ratio of 15, with ex-situ ozone only (no UV irradiation) and a stage temperature of 100°C, the polyimide samples did not show a significant ashing rate or contact angle decrease. However, at 200°C, the samples processed with ex-situ ozone only (no UV irradiation) showed contact angle of 15.40° against the initial value of 93.70° and an ashing rate of 9.95 nm/min. The samples processed using UV irradiation with ex-situ ozone at 200°C showed a contact angle of 75.93° and an ashing rate of 7.67 nm/min.

From these results, it was concluded that production of oxygen radicals was accelerated by thermal dissociation of ozone at the higher temperature. The oxygen radical flux produced at high temperature gradually decreased in the cave as the aspect ratio became greater, but it remained relatively high and caused temperature-driven surface chemical reactions. It was postulated that the 254 nm UV irradiation dissociated ozone that otherwise would have reached deep inside the cave and thermally dissociated [2].

[1] Uehara, S., Kawabe, T., Wood, P., & Tsuji, O. (2016). *MRS Advances,* **1**.11, 743-748.

[2] Wood, P., Wydeven, T., & Tsuji, O. (1993). *MRS Proceedings,* **315**. 237.

5:20pm **SS+AS+EM-ThA-10 Density Functional Theory Study of the Effects of Surface Defects on the Interactions of Cl and α-$Fe_2O_3$ (0001) Surface**, ***Qin Pang**, H DorMohammadi, O Isgor, L Árnadóttir,* Oregon State University

Fe (III) oxides are the dominant structure of the outer layer of the iron passive film formed in alkaline environment, but chloride ions have been shown to induce depassivation of these passive films under the same conditions. Here we use hematite (α-$Fe_2O_3$) to represent the Fe (III) oxides and DFT+U method to investigate the mechanism of the depassivation by studying the interactions of Cl with both pristine α-$Fe_2O_3$ (0001) surface and the surface with defects. Total of four surfaces are considered, pristine surface, Fe vacancy surface, O vacancy surface and Fe-O pair vacancy surface. We found that the O vacancies have a positive effect on the adsorption of Cl on the surfaces while the Fe vacancy has a negative effect. The strength of the adsorption on the same site on the four surfaces can be ranked as O vacancy surface, Fe-O pair vacancy surface, pristine surface and Fe vacancy surface. The insertion of the Cl into the sub surface was studied on the four surfaces as well and was found to be endothermic for all four surfaces but surface defects have positive effects on the insertion of Cl by making it less endothermic. The insertion reaction is less endothermic on the O vacancy surface and Fe-O pair vacancy surface. On these two surfaces, the Cl insertion process goes through an O vacancy with reaction energy around 0.5 eV, which is about 1 eV lower than the reaction energy on the pristine surface. The Cl insertion energy is slightly coverage depended, but the insertion remains less favorable than the adsorption of Cl even at higher coverages.

## Electronic Materials and Photonics Division
## Room Central Hall - Session EM-ThP
## Electronic Materials and Photonics Poster Session

**EM-ThP-3 Electrolyte-Insulator-Semiconductor (EIS) device with Different Integrated Reference Electrodes for pH Detecting***, **Rodrigo Reigota**, J Diniz,* University of Campinas (UNICAMP), Brazil

In this work Electrolyte-Insulator-Semiconductor (EIS) device has been developed for pH measurements. This device operates as a Metal-Oxide-Semiconductor capacitor but instead of having the metal contact electrode, an electrolyte solution and a reference electrode are used to apply voltage. Titanium nitrite (TiN), aluminium (Al) and alumina/aluminium ($Al_2O_3$/Al) were used as reference electrode integrated with EIS device. These materials were deposited by DC sputtering. As dielectric material and sensitive membrane was chosen titanium dioxide ($TiO_2$). This film was obtained by DC sputtering, and was structurally characterized by Atomic Force Microscopy, Raman and Ellipsometry. The structural characterization of $TiO_2$ thin film shows the presence of rutile and anatase crystal structure, physical thickness of 50 nm, refractive index of 2.44 and roughness of 0.4 nm. Was developed MOS capacitors to make the electrical characterization of $TiO_2$ thin films in order to determine the annealing time that leads to the best thin film properties, defined by high dielectric constant value (high-k), lower charge density ($Q_0/q$) and flat-band voltage ($V_{FB}$) around -0.9V. The electrical characterization done by Capacitance x Voltage (CxV) curves revealed that with 15 min annealing the films exhibit the best dielectric constant equals to 133 which is higher than reported in literature. The $V_{FB}$ was -0.6V and $Q_0/q$ in the order of $-10^{+12}/cm^2$. The Current x Voltage (IxV) curve shows that the current through the dielectric is approximately $1x10^{-9}$A. With dielectric characterized it was possible to develop the EIS device. From electrical characterization it was possible to test the integrity of the electrodes and determined the sensitivity of the device. For electrical measurement of EIS was used Normalized Capacitance x Voltage curve (CxV curve) using different pH (4, 7 and 10) solutions. From the flat band voltage ($V_{FB}$) of the Normalized CxV curves was possible to determine the sensitivity of the device. The Al and $Al_2O_3$/Al reference electrodes showed a low acid resistance. After measurement with pH 4 the electrodes were corroded. The TiN reference electrode showed to be a very resistant material. This electrode supported the electrical measurements with the three solutions. However, the EIS with the TiN reference electrode showed a low sensitivity of 20mV/pH.

**EM-ThP-4 Optical and Magneto-optical Properties of $Zn_{1-x}Co_xO$ / ZnO Hollow Nanospheres***, **Da-Ren Liu**, C Weng,* Instrument Technology Research Center, National Applied Research Laboratories

Diluted magnetic semiconductors (DMS) have attracted considerable attention due to their potential applications for spintronic devices, such as spin-valve transistors, nonvolatile memory, and magneto-optical switches. ZnCoO is one of the most promising DMS materials due to its predicted above room temperature ferromagnetism. In this study, ZnO layer was conformally deposited on the surface of polystyrene (PS) nanoshperes with different diameter (100nm~800nm) by atomic layer deposition (ALD). Then the $Zn_{1-x}Co_xO$ ($0.01 < x < 0.1$) coatings were grown on ZnO hollow nanospheres by pulsed laser deposition(PLD). According to the results of high-resolution x-ray diffraction, Co-doping does not change the wurtzite structure of ZnO and the $Zn_{1-x}Co_xO$/ZnO hollow nanospheres are polycrystalline. Photoluminescence spectra and transmittance show an increase of the band gap with increasing Co ion concentration. The temperature-dependent magnetization (M-T) curves of the $Zn_{1-x}Co_xO$/ZnO hollow nanospheres were measured by a superconducting quantum interference device (SQUID) magnetometer and the magneto-optical properties were measured by micro-MOKE spectroscopy. The results show the magneto-optical properties of the $Zn_{1-x}Co_xO$/ZnO hollow nanospheres depend on the Co composition fraction and the size of nanospheres.

**EM-ThP-5 Low-k Cryo-etching: Comparison of Four Different High Boiling Point Organic (HBPO)***, **Romain Chanson**,* IMEC, Belgium*; P Lefaucheux, R Dussart, T Tillocher,* GREMI, France*; P Shen, K Urabe, C Dussarat,* Air Liquide, Japan*; K Maekawa,* TEL Technology Center, America, LLC*; K Yatsuda,* Tokyo Electron Limited, Japan*; S Tahara,* Tokyo Electron Miyagi Limited, Japan*; J de Marneffe,* IMEC, Belgium

Low temperature plasma processing is investigated for low damage etching of porous organo-silicate glass ultra-low-k (p-OSG) dielectrics. For additional film protection, in-situ micro capillary condensation is used. This effect allows condensation of a gas precursor into the porous structure. The condensate densifies the porous structure and avoids the plasma by-products to react with the $Si-CH_3$ terminating bonds. In this work, high boiling point organic (HBPO) molecules are studied as reagents for pore filling, enabling for the different gas condensation from -20°C to -50°C. The micro-capillary condensation properties of selected molecules in p-OSG will be compared as well as their desorption kinetic and stability when exposed to a pure $SF_6$ plasma. Using the most promising reagent, patterning tests using a 45nm ½ pitch vehicle and k=2.2 periodic mesoporous oxide low-k dielectric allows to generate vertical trench profiles with good mask selectivity (TiN). A slow kinetic of desorption and a large “Working Window” are critical points for optimal low-k protection.

Acknowledgement: We would like to acknowledge the European commission for its financial support.

**EM-ThP-6 Carrier Ion Exchange of $Na_2O-Fe_2O_3-P_2O_5-SiO_2$ Glass-Ceramics***, **Yoshikazu Kaji**, N Yoshida, T Okura,* Kogakuin University, Japan

Our group has developed $Na^+$-superionic conductive Narpsio (typically represented as a general formula of $Na_3RP_ySi_{3-y}O_9$, R=rare earth) glass-ceramics, as analogues of $Na_5RSi_4O_{12}$ (N5)-type $Na^+$-superionic conductors, and it was revealed that these showed excellent ionic conductivity up to ~$10^{-1}$ S/cm, which is comparable to those of the conventional ceramic $Na^+$-conductor such as b- and b²-aluminas and NASICONs. Recently we achieved two important replacements, that is, R with Fe, and carrier $Na^+$ with $H^+$. The replacement of R with cheap and rich Fe is important in terms of cost and amounts of resources. The carrier ion exchange of $Na^+$ with $H^+$ will spread its applications, such as a fuel cell.

In this study, $Na_{4.9}FeP_{0.1}Si_{3.9}O_{12}$ glass-ceramics of N5 phase was prepared at first, and then, exchange of carrier $Na^+$ ion with $H^+$ was tried in several conditions.

$Na_{4.9}FeP_{0.1}Si_{3.9}O_{12}$ glass-ceramics of N5 phase was prepared by melt-quenching and glass-crystallization method. Ion exchange experiment was carried out as follows; while monitoring with pH meter, prepared glass-ceramics was immersed into HCl aq. with/without NaCl at room temperature.The obtained samples were characterized by X-ray diffraction analyses (XRD), thermogravimetry-differential thermal analysis (TG-DTA), differential scanning calorimetry (DSC).

XRD measurement indicated that glass-ceramic $Na_{4.9}FeP_{0.1}Si_{3.9}O_{12}$ of N5 phase was successfully prepared. After ion exchange without addition of NaCl, unknown phase was appeared in XRD pattern, and this change could not be suppressed by changing concentration of HCl aq. A possible explanation against this change is due to dissolution of bonding $Na^+$ in addition to carrier $Na^+$. After ion exchange with addition of NaCl, unknown phase was disappeared, although slight decrease in crystallinity was observed.

Glass-ceramic $Na_{4.9}FeP_{0.1}Si_{3.9}O_{12}$ of N5 phase was successfully prepared and replaced carrier $Na^+$ ion with $H^+$ without significant changes in crystallinity under the conditions of ion exchange with addition of NaCl. Detail of experiments and thermodynamic data will be discussed in the presentation.

**EM-ThP-7 Defect Doping ZnO Thin-Films with γ - Radiation***, **Seth King**, K Slezak,* University of Wisconsin - La Crosse*; S Chamberlin,* Lawrence University*; S Lantvit,* University of Wisconsin - La Crosse

Sputter deposited ZnO thin films have been exposed to prolonged high energy gamma radiation in a 400 Ci $^{137}Cs$ irradiator to examine the impact of such exposure on the optical, structural, and electronic properties of this technologically important wide-bandgap semiconductor . While many studies have shown that ZnO is radiation hard to proton and electron damage [1,2], only one has investigated the effects of exposure to high-energy photons, and not in an iterative manner [3].

UV-Vis spectrometry and spectroscopic ellipsometry show little variation in the over-all transmittance, optical constants, or optical bandgap of the irradiated films. Continued exposure shows a decrease in the films' resistivity, which, along with supporting x-ray photoelectron spectroscopy data, suggests that induced O-vacancies are acting as donors to dope the irradiated films.

References:

1) S.O. Kucheyev, J.S. Williams, C. Jagadish, J. Zou, C. Evans, A.J. Nelson, and A.V. Hamza, Ion-beam-produced structural defects in ZnO, *Phys. Rev. B*, 67, **2003**, 094115

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3)N. A. Al - Hamdani, R.D. Al – Alawy, and H.J. Hassan, *Jrnl. Comp. Eng.*, 16, **2014,** 11-16

### EM-ThP-8 Design and Synthesis of Precursors for Photoassisted Chemical Vapor Deposition

***Christopher Brewer**, O Hawkins,* University of Florida*; B Salazar, A Walker,* University of Texas at Dallas*; L McElwee-White,* University of Florida

Chemical vapor deposition (CVD) is a potentially attractive technique for the metallization of organic thin films. However, thermal CVD processes often require high temperatures which are incompatible with organic substrates. Photochemistry provides an alternative means of initiating precursor decomposition without heating the substrate. Readily available Ru precursors, including ($\eta^3$-allyl)Ru(CO)$_3$X and CpRu(CO)$_2$X (X = Cl, Br, I), have been used to deposit Ru on functionalized self-assembled monolayers (SAMs) by means of photochemical CVD as a model system for deposition of metal on a thermally sensitive substrate. Carboxylic acid-, hydroxyl- and methyl-terminated SAMs were used to explore the effects of surface functionality on deposition and the presence of Ru on the SAMs was confirmed by HR TOF SIMS. Preliminary experiments have shown that an attractive precursor for photoassisted CVD will be volatile, have an acid sensitive functionality and have a reasonable quantum yield for ligand loss. Synthesis of the precursors, determination of the quantum yields and deposition of Ru onto the functionalized SAMs will be discussed.

### EM-ThP-9 Electrical and Mechanical Improvements with a Non-Thermal Curing Process for Porous SiCOH using Combined Ultraviolet and Vacuum-Ultraviolet Radiation

***Sang-heum Kim**, J Blatz, W Li, H Zhang, D Pei, T Guo, X Zhou,* University of Wisconsin-Madison*; Y Lin, H Fung, C Chen,* National Synchrotron Radiation Research Center, Taiwan, Republic of China*; S King,* Intel Corporation*; Y Nishi,* Stanford University*; J Shohet,* University of Wisconsin-Madison

Porous SiCOH films are rapidly emerging as preferred interplay dielectric materials in semiconductor fabrication because of their ultra-low dielectric-constant properties. Ultraviolet (UV) light on organosilicate thin films in post-deposition treatments initiates to photo-chemical process by nano pores generators (porogens) and form a network to improve mechanical properties of the dielectrics. A simple and cost-saving method of improving not only the mechanical property but also electrical property was found by combined with two different UV exposure energies called UV/Vacuum Ultraviolet (VUV) photons curing without the need for heating the dielectric [1] The goal of this work is to choose the best combined UV/VUV photon energies and to investigate beneficial effects that lower the dielectric constant, minimize damage, and increase the elastic modulus of low-k dielectrics as a function of the fluence of the UV/VUV curing photons. The following measurements were made. (1) We exposed SiCOH films samples with UV/VUV photon energies ranging from 4.5 to 8.9 eV from a beamline at the National Synchrotron Radiation Research Center (NSRRC) in Taiwan. (2) Using both nanoindentation and Time-Dependent Dielectric Breakdown (TDDB) measurement, we found the most beneficial energies (usually 2) for improving both electrical and mechanical properties could be found from VUV spectroscopic measurements. (3) We exposed the same SiCOH films at the same beamline using two combined photon energies with four different fluences from 5 x 10^14 photons/cm2 and 10^16 photons/cm2. (4) We measured TDDB and the nanoindentation after exposure. We show that this method can be applied to different porous SiCOH films, so that we can overcome drawbacks of UV curing and improve the properties of these dielectrics at room temperature.

This work was supported by the Semiconductor Research Corporation under Contract No. 2012-KJ-2359.

[1] H. Zheng, *et al.Applied Physics Letters*, **108** 242906. (2016)

### EM-ThP-10 The Effects of Cesium Ion Implantation on the Mechanical and Electrical Properties of Porous SiCOH Low-k Dielectrics

***Weiyi Li**, D Benjamin, J Chang,* University of Wisconsin - Madison*; Q Lin,* IBM Research Division, T.J. Watson Research Center*; S King,* Intel Corporation*; J Shohet,* University of Wisconsin - Madison

In this work, we investigate the effects of cesium (Cs) ion implantation on both porogen-embedded and UV-cured (porous) SiCOH films. It has been shown in past work that Cs doping has benefits for either spin-on low-*k* dielectrics[1] or PECVD deposited non-porous SiCOH low-*k* dielectrics.[2] For porogen-embedded SiCOH, it was found that Cs ion implantation can greatly improve the elastic modulus up to twice its original value . It can also increase the time-zero dielectric breakdown (TZDB) strength. It also leads to an increase in the k-value for medium and high Cs doses, but for low Cs doses the k-value decreases compared with its pristine counterpart. These effects can be understood by examining the changes in Si-CH$_3$ bonds and Si-O bonds . For UV-cured SiCOH, it was found that Cs ion implantation does not modify the elastic modulus. This also leads to lower TZDB field strength and much higher k-values than its pristine counterpart. This treatment is shown to have a potential to help solve the problem between the demand for lower k-values and the concomitant weak mechanical strength of SiCOH.

This work was supported by the Semiconductor Research Corporation under contract 2012-KJ-2359.

[1] W. Li, D. Pei, X. Guo, M. K. Cheng, S. Lee, Q. Lin*, et al.*, "Effects of cesium ion-implantation on mechanical and electrical properties of organosilicate low-k films," *Applied Physics Letters,* **108**, 202901, (2016).

[2] Y. Kayaba, K. Kohmura, H. Tanaka, Y. Seino, T. Odaira, F. Nishiyama*, et al.*, "Electrical reliabilities of highly cross-linked porous silica film with cesium doping," *Journal of the Electrochemical Society,* **155**, G258 (2008).

### EM-ThP-11 The Effect of Proton Radiation on ALD HfO$_2$ Films and HfO$_2$ base RRAM

***Panpan Xue**,* University of Wisconsin-Madison*; Z Wang,* Stanford University*; T Chang,* University of Wisconsin-Madison*; Y Nishi,* Stanford University*; J Shohet,* University of Wisconsin-Madison

Hafnium oxide(HfO$_2$) is one of the most popular dielectric materials for RRAM. Changes of the defect concentrations of HfO$_2$ may affect the resistive-switching mechanism of RRAM. In this work, in order to investigate the effects of proton radiation, (1) atomic-layer-deposited (ALD) HfO$_2$ blanket films deposited on a Si substrate and (2) HfO$_2$ base RRAM were exposed to proton. After exposure, electron spin resonance and FTIR measurements were made on the HfO$_2$ blanket film, forming voltage and I-V characteristics were measured on the RRAM cell. The samples were exposed to proton radiation with a range of energies from 10 to 300keV. H ion implantation was used as the proton source. ESR measurements showed that after 300keV proton exposure, the defect concentration of Si dangling bond increased. Besides, all of the fresh pristine RRAM cells need to be formed, the forming voltage is approximately 3.4 ~ 3.65V. However, a number of the low-energy proton-exposed samples are set after exposure: about 50% of the 10keV proton exposed RRAM samples are set to the “on” state after irradiation. The 300keV proton-exposed RRAM samples were not formed or set after proton exposure, but the needed forming voltage decreased and breakdown occurred at a lower voltage. This is consistent to a TRIM simulation result, after low energy exposure, some of the H ions are seen to stay in the HfO$_2$ films and generate conductive filaments that set the dielectric film to the low resistance state. However, 300keV protons have just enough energy to pass through the dielectric film. In addition, the high-resistance state (HRS) current of just-formed 300keV exposed RRAM is about 100 times higher than that for pristine RRAM. We conclude low-energy protons have a significant effect on the forming process of RRAM. However, higher-energy protons change the resistance of the HRS instead.

This work was supported by the Semiconductor Research Corporation under Contract 2012-KJ-2359

### EM-ThP-12 Measurement of the Depth of Plasma Damage caused by VUV Photons and Oxygen Radicals using X-ray Reflectivity

***Ha Nguyen**, F Choudhury,* University of Wisconsin-Madison*; C Lee,* National Tsing Hua University, Taiwan, Republic of China*; Y Lin, H Fung, C Chen,* National Synchrotron Radiation Research Center, Taiwan, Republic of China*; J Blatz, D Benjamin, W Li, J Shohet,* University of Wisconsin-Madison

During plasma processing, dielectric films used in the semiconductor technology are often exposed to large doses of vacuum ultraviolet (VUV) radiation and free radicals that can damage the dielectric material. In this work, we utilize specular x-ray reflectivity to measure the depth of damage of dielectric films as a function of energy of VUV photons and various doses of oxygen radicals. First, we examine the VUV-absorption spectrum of low-k organosilicate glass (OSG) using specular X-ray reflectivity (XRR). Low-k SiCOH films were exposed to synchrotron VUV radiation with energies ranging from 7 to 25 eV and the density depth profile of the VUV-irradiated films were extracted from the fitting of the XRR experimental data. The results show that the depth of the VUV-induced damage layer is a function of photon energy. Between 7 and 11 eV, the depth of the damaged layer decreases sharply from 110 nm to 60 nm and then gradually increases to 85 nm at 21 eV. The maximum VUV absorption in the OSG films occurs between 11 and 15 eV. Next, SiO$_2$ dielectric films were exposed to oxygen plasma in an electron cyclotron resonance plasma reactor and XRR measurements were made in order to determine the depth of damage as a function of oxygen-radical dose. It was found that the depth of damage increases as a function of plasma exposure time and eventually saturates to ~ 66 nm after about 30 minutes of oxygen-plasma exposure. This work shows that XRR damage depth profiling can be a very effective, non-destructive tool to determine the penetration depth of VUV photons and other plasma reactive species in dielectric films [1].

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[1] Faraz A. Choudhury *et al*. "Oxygen radical transmission through and damage to freestanding single and multilayer dielectric films" AVS 64th International Symposium & Exhibition, Tampa, Florida (2017).

**EM-ThP-13 Oxygen Radical Transmission through and Damage to Freestanding Single and Multilayer Dielectric Films***, **Faraz Choudhury**, G Sabat, M Sussman,* University of Wisconsin-Madison*; Y Nishi,* Stanford University*; J Shohet,* University of Wisconsin-Madison

During plasma processing, dielectric films are exposed to a high concentration of free radicals that can affect the processing conditions and the properties of materials exposed to the plasma. Measuring the absorption lengths and penetration depths of free radicals is critical in order to determine their effects on the dielectric materials. Using radical-sensitive fluorescent dyes and free-standing films, the transmission of oxygen radicals through silicon nitride and silicon dioxide dielectric films is measured. The absorption length of the oxygen radicals is determined by measuring the number of transmitted radicals as a function of the thickness of the freestanding films. For silicon nitride films, the absorption length was found to be 33 nm for 15-minute oxygen plasma exposure. The absorption lengths increased to 37 and 40 nm for 30 minute and 45-minute plasma exposures, respectively. FTIR measurements showed a decrease in Si-N bond concentration after plasma exposure and a subsequent appearance of Si-O-Si bonds. In addition, the density vs. depth profiles of the pristine and plasma exposed films were obtained from specular x-ray reflectivity (XRR) measurements which showed that the plasma exposure forms a silicon oxynitride-like layer on the surface of the film which has a lower density than silicon nitride. The increase in absorption length with plasma-exposure time is attributed to the formation of the surface layer. In silicon dioxide films, the absorption length of oxygen radicals was found to be ~70 nm after 20 minutes of plasma exposure. After 30 minutes of plasma exposure under the same conditions, the absorption length was reduced to ~66 nm. XRR and FTIR measurements both reveal that the oxygen plasma exposure leads to further oxidation of the silicon dioxide film and the formation of a denser surface layer which restricts the transmission of the radicals through the film.

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**EM-ThP-15 Effect of Proton Irradiation on Device Characteristics of Bottom Gate ZnO Thin Film Transistors with Sol-Gel Derived Channel Layers***, **Kosala Yapabandara**, V Mirkhani, S Wang, M Khanal, S Uprety,* Auburn University*; M Sk,* Qatar University, Qatar*; A Ahyi, T Isaacs-Smith, M Hamilton, M Park,* Auburn University

ZnO has been widely studied due to its promising material properties as a wide energy bandgap semiconductor, optical transparency, and high carrier mobility for thin film transistor (TFT) technology. Solution-based ZnO can easily be deposited on large areas of substrates at low temperatures, which makes this material a good candidate for commercial device manufacturing. Moreover, ZnO exhibits a higher radiation hardness compared to semiconductors such as Si, GaAs, and GaN. However, it is not entirely understood why ZnO shows superior radiation hardness over GaN.

In this work, we report the device performance analysis of solution derived ZnO TFTs upon irradiation of 100 keV proton with $10^{14}$ $cm^{-2}$ fluence. A comprehensive analysis of unirradiated and irradiated samples was performed to elucidate the proton irradiation effect on ZnO TFTs. The room temperature photoluminescence analysis showed a slight reduction in intensities of near-band-edge UV peak and visible luminescence band while the peak positions and the full-width half maximum (FWHM) are unchanged upon irradiation. This implies that negligible damage has occurred in the ZnO channel layer due to the proton irradiation. From transfer characteristics analysis, it was observed that the reduction in the drain current ($I_D$) at high drain-source voltages ($V_{GS}$) regime is less than an order of magnitude, which also suggests minimal irradiation damage to the ZnO lattice. However, the shift in $V_{ON}$ and an enhancement in subthreshold swing (SS) after the proton irradiation were observed, which is believed to be produced by radiation-induced electron-hole pair production in the $SiO_2$ layer. Multiple peaks in incremental mobility ($\mu_{inc}$) variation with $V_{GS}$ and a plateau in low-frequency C-V curve were observed in unirradiated samples. A model was proposed to explain these abnormalities. It is reasonable to think that a significant number of defects is introduced into sol-gel derived ZnO channel during the deposition process. Since our deposition process requires more that one spin coating run, ZnO-ZnO interlayer interfaces will be formed. It was hypothesized that the depletion regions are created by oxygen-related trap centers at the ZnO-ZnO interlayer interfaces. It was conjectured that the disappearance of multiple peaks in $\mu_{inc}$ and the plateau in low-frequency C-V curve upon proton irradiation might be the result of the reduction of the depletion layer in the proximity of ZnO-ZnO interlayer interface.

**EM-ThP-16 Characterization of the Buried MgO/Al Interfaces in Multilayer Heterostructures used as Photocathodes with Hard X-ray Photoelectron Spectroscopy***, **Jeff Terry**,* Illinois Institute of Technology

Early research and development of photocathode material was based on characterizing compounds with low work function and high quantum efficiency. Recent theoretical and experimental work has shown that the metal-insulator junctions can give rise to changes in the band structure at the interface, which in turn leads to a change in work function and quantum efficiency.

In addition to concerns about work function and quantum efficiency, many modern photoinjector designs also require low beam emittance. Beam emittance is an intrinsic property of the photocathode, therefore it is important to be able control the growth and quantify the factors that lead to such growth. Nemeth [Phys. Rev. Lett. 104, 046801 (2010)] used DFT to model metal- insulator multilayer junction. The model indicate that it is possible to reduce the emittance of the photoemitted beam. Velazquez et al [Appl. Surf. Sci. 360, 762 (2016)] has demonstrated that the work function of lab grown thin film multilayers had trends that match the theory. However the model predicted an exponential decrease of work function, but data suggests a linear decrease.

It has been suggested that the surface roughness of the lab grown thin film multilayers might be the main cause of the deviation from the theory. Thin films are synthesized with a custom build dual laser PLD system, and the surface roughness is systematically altered by growing at different substrate temperature. We utilized a Hard X-ray Photoelectron Spectroscopy (HAXPES) system on the MRCAT undulator beamline at the Advanced Photon Source to characterize the MgO/Ag multilayers to better understand the chemistry at the interface. Understanding the reactivity, can help us better understand how the growth transitions from uniform to rough with increasing layer number.

**EM-ThP-17 Gamma-Ray Irradiation Effects on HfO2 RRAM Studied via EDMR***, **Duane McCrory**, P Lenahan,* Penn State University*; D Nminibapiel, D Veksler, J Ryan, J Campbell,* National Institute of Standards and Technology

Resistive Random Access Memory (RRAM) is a leading candidate for future non-volatile memory applications. These devices may be extremely useful for space applications. However, at the present time there is virtually no direct experimental evidence identifying the atomic scale defects involved in RRAM radiation damage or the underlying atomic scale conduction mechanisms. One of the most promising systems for RRAM is $HfO_2$ metal-insulator-metal based devices. In these devices, it is believed that the switching mechanism is derived from filamentary conduction paths within the oxide. One widely accepted mechanism involves the migration of oxygen vacancies within the transition-metal-oxide insulator, forming the conducting filament [1]. However, to the best of our knowledge, no direct experimental evidence establishes this transport mechanism.

By far the most powerful analytical tool available for identifying atomic scale defects is electron paramagnetic resonance (EPR). Using conventional EPR, Ryan et. al. have identified two atomic scale defects directly involved in gamma-irradiation damage; an $O^{2-}$ coupled to a hafnium ion, and an oxygen vacancy center [2]. However, conventional EPR is not sensitive enough to observe defects within the RRAM. We must look elsewhere to identify the defects and transport mechanisms. The most sensitive technique for identifying these defects is electrically detected magnetic resonance (EDMR) [3].

In this study we have subjected the $TiN/Ti/HfO_2/TiN$ RRAM devices to 1 MRAD of $^{60}Co$ gamma irradiation. These 100x100 nm devices are cross-point type RRAM with 5nm thick $HfO_2$. We have made EDMR measurements before and after gamma irradiation. We observe the radiation induced generation of two strong spectra that appear in both the in-phase and quadrature. We believe that this response is due to two different trap assisted tunneling mechanisms within the oxide. Both spectra appear to be reasonably consistent with the earlier observations of

Ryan et. al [2]. A DFT study by Muñez et. al. linked this defect earlier observed for the Ryan et. al. as an oxygen vacancy [4]. DFT calculations by Bradley et. al. have linked two di-vacancy sites near the middle of the $HfO_2$ bandgap that may contribute to transport in $HfO_2$ [5]. Our results provide strong evidence linking electronic transport and radiation damage mechanisms to transport through oxygen vacancy related centers.

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**EM-ThP-19 Defect Dependent Luminescence Dead Layers in CdS and CdSe**, ***Richard Rosenberg***, Argonne National Laboratory

CdS and CdSe are often used in optoelectronic devices whose effectiveness may be dictated by defects in the near surface region. Luminescence is one of the main tools for studying such defects. The energy dependence of the X-ray excited optical luminescence (XEOL) spectra of these materials enables the extraction of the depth-dependence of the defect distribution.[1] Normal and time-gated XEOL spectra were obtained from these materials in the X-ray energy range 600 to 1500 eV. The individual components of each spectrum were extracted using curve fitting techniques. Each component's energy-dependent intensity was fit to a "dead layer" model.[2] We find that the results can best be understood in terms of a luminescence dead layer whose width depends on the position of the defect level in the band gap.

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**EM-ThP-20 High Breakdown Voltage (-201) β-$Ga_2O_3$ Schottky Rectifiers**, ***Jiancheng Yang**, S Ahn, F Ren, S Pearton,* University of Florida

A reverse breakdown voltage of 1600 V was demonstrated for Schottky diodes without edge termination fabricated on 10 µm epitaxial β-$Ga_2O_3$ grown bulk conductive substrate. $Ga_2O_3$ has a theoretical Baliga figure of merit (defined as $V_B^2/R_{ON}$, where $V_B$ is the reverse breakdown voltage and $R_{ON}$ is the on-state resistance) significantly higher than more familiar wide bandgap semiconductors, due mainly to its larger bandgap (~4.5-4.8 eV) compared to that of 4H or 6H-SiC and GaN (~3.0-3.4 eV). The theoretical breakdown electric field is ∼8 MV/cm, with experimental demonstrations as high as 3.8 MV/cm and this is already higher than the bulk critical field strengths of both GaN and SiC. In this work, the β-$Ga_2O_3$ Schottky barrier diodes were fabricated in a vertical geometry structure consisting of Ni/Au rectifying contacts without edge termination on Si-doped epitaxial layers (10 µm, n~ $4\times10^{15}$ $cm^{-3}$) grown on Sn-doped bulk $Ga_2O_3$ substrates with full area Ti/Au back Ohmic contacts. The reverse breakdown voltage, $V_{BR}$, was a function of rectifying contact area, ranging from 1600V at $3.1\times10^{-6}$ $cm^2$ (20µm diameter) to ~250V at $2.2\times10^{-3}$ $cm^{-2}$ (0.53 mm diameter). The current density near breakdown was not strongly dependent on contact circumference but did scale with contact area, indicating the bulk current contribution was dominant. The lowest on-state resistance, $R_{on}$, was 1.6 mΩ-$cm^2$ for the largest diode and 25 mΩ.$cm^2$ for the 1600V rectifier, leading to a Baliga figure-of-merit ($V_{BR}^2/R_{on}$) for the latter of approximately 102.4 MW·$cm^{-2}$. The on-off ratio was measured at a forward voltage of 1.3V and ranged from $3x10^7$ to $2.5x10^6$ for reverse biases from – 5 to -40 V and showed only a small dependence on temperature in the range 25-100°C. The Schottky barrier height decreased from 1.1 at 25°C to 0.94 eV at 100°C, while the ideality factor increased from 1.08 to 1.28 over the same range. The reverse recovery time was 26 ns for switching from +5V to -5V. These results represent another impressive advance in the quality of bulk and epitaxial β-$Ga_2O_3$.

**EM-ThP-21 Inelastic Electron Tunneling Spectroscopy and Electron Conduction Mechanisms of Porphyrin Molecular Junctions**, ***Teresa Esposito**, P Dinolfo, V Meunier, K Lewis,* Rensselaer Polytechnic Institute

In order to achieve nanoscale electronic devices beyond the 10 nm limit predicted by Moore's Law, molecular electronic devices are being studied as alternatives to circuit elements such as diodes, switches, and transistors. Porphyrin molecules are of interest because they have been shown to exhibit switching and diode behavior. In addition, shorter porphyrins (2-3 nm) can be used as interconnects because their low attenuation factors (β<0.01 $nm^{-1}$) allow for long range electron conduction. Our work investigates three types of short porphyrins: a free base porphyrin, and porphyrins with either a zinc or an iron atom ligated to the porphyrin ring. Nanostructures are formed by depositing porphyrins into a 3-5 nm gap created by electromigration of a 30x50 nm gold nanowire to create a molecular junction (MJ). In order to determine the mechanism for electron conduction through these porphyrin MJs, temperature dependent current-voltage (I/V) studies have been performed and compared to existing models of electron transport, and are shown to be direct tunneling. Inelastic electron tunneling spectroscopy (IETS), which is the second derivative of I/V, is measured simultaneously at temperatures from 4.2 to 300 K. IETS is used to verify the presence of a molecule in the gap. Peaks in the spectra indicate the excitation of a vibrational mode, which are compared to Fourier transform infrared spectroscopy, surface enhanced Raman spectroscopy, and theoretical density functional theory calculations.

**EM-ThP-22 Welding of Metal Nanowire Networks Using Eddy Current Method**, ***JiSoo Oh**, D Sung, D Kim, K Kim, G Yeom,* Sungkyunkwan University, Republic of Korea

Silver nanowire (AgNW) network is one of the most promising candidates to replace indium tin oxide (ITO) as transparent conductors among several candidates such as carbon nanotubes, graphene, metal grid, conducting polymer, etc. AgNW has lots of advantages, for example, AgNW not only has inherent high electrical conductivity and high transparency but also can be easily fabricated by using various methods on the flexible substrates. Despite these advantages, AgNW has its limitations due to high surface roughness and low adhesion problem. Especially, a high contact resistance between AgNW from the coating of polyvinylpyrrolidone (PVP) due to the loose contact between individual AgNWs is a critical issue to be resolved.

In order to overcome these problems, we constructed an inductive coil system that generates eddy current and welded nanowires with different operating frequencies. This method welds only the junction between the nanowires without heating the substrate due to higher resistance at the junction. Using this method, the various metal nanowires such as Ag and Cu nanowires were successfully welded by reducing the sheet resistance about 67% without changing the optical transmittance, and it was confirmed that it can be applicable to various flexible dielectric substrates such PET substrates. Due to the local melting at the junction, the decrease of surface roughness could be also confirmed by surface image measurement. In addition, no significant change in resistance by bending test and adhesive test was observed due to the successful welding of the junction part of the nanowire, thereby improving the properties of the nanowire networks. This welding method is believed to be applicable to all kinds of metal nanowires without heating or touching of the substrate and on a large area at short process time and at low-cost.

**EM-ThP-23 Deep Ultraviolet Light Source with Carbon Nanotube based Electron Beam Pumping**, ***KyuChang Park**, S Yoo,* Kyung Hee University, Republic of Korea

Deep ultaviolet (UVC) light sources were fabricated with carbon nanotube based electron beam pumping technique. Anode materials for UVC generation made by home-made fabrication process with Zn & Si mixture and irradiated with the carbon nanotube based cold cathode electron beam (C-beam). The C-beam fabricated with triode structure with metal mesh gate electrode and CNT cold cathode. The C-beam shows more than 90% electron transmittance through gate electrode and more than 10 mA anode current in DC operation.

For UVC light generation, anode semiconducting layer formation process is very important and should be optimized with electron beam irradiation current density. The UVC light intensity strongly related on the annealing conditions of anode layer and optimized to 1,000 degree celcius and nitrogen ambient. To reduce the power consumption, C-beam irradiated with DC pulse driving.

UVC light source with novel anode and C-beam irradiation technique shows emission peak at 208 nm, 226 nm, and 245 nm. The emission peak depend on the anode fabrication process and C-beam irradiation coditions. More detail on the UVC light fabrication with C-beam irradiation will be presented

### EM-ThP-24 An Unexpected Trend between Metal Work Function and Contact Resistance to Germanium Telluride

***Kayla Cooley***, *H Simchi, H Aldosari, J O'Neil, S Yu, A Molina, S Mohney,* The Pennsylvania State University

Germanium telluride is an emerging phase change material (PCM) that has shown exceptional promise for radio frequency (RF) switch technology. When an appropriate heating schedule is applied, this material quickly transitions between crystalline (conductive ON state) and amorphous (highly resistive OFF state). Currently, the contact resistance ($R_c$) contributes 20-50% of the ON-state resistance of the switch and significantly degrades RF circuit performance. Low-resistance Ohmic contacts that are able to withstand the thermal cycling necessary for changing the phase of GeTe are therefore necessary for successful implementation of GeTe-based RF switches .

We investigated selected contact metals (Ti, Sn, Cr, Mo, Ni, Au, and Pt), resulting in $R_c$ from 0.004 to 0.036 Ω-mm (specific contact resistances of $5 \times 10^{-9}$ to $4 \times 10^{-7}$ Ω-cm$^2$) . We also characterized surfaces and interfaces using X-ray photoelectron spectroscopy and transmission electron microscopy with energy dispersive spectroscopy. The lowest $R_c$ values (0.004 ± 0.001 Ω-mm) were achieved using Sn and Mo-based contacts, with $R_c$ ranked according to the first metal deposited as follows: Mo or Sn < Cr < Ti < Au < Ni < Pt. This trend is surprising, as high work function metals, like Au and Pt, would be expected to provide lower $R_c$ values to *p*+ GeTe.

In the case of Sn-based contacts, low $R_c$ can be attributed to a beneficial interfacial reaction that formed SnTe upon deposition at the contact interface; however, for Mo-based contacts, no such interfacial reaction was observed. Chemical reactions at the interface were not always favorable. In the case of Pt and Ni, the formation of metal tellurides resulted in very high $R_c$. Thermal stability of all contact metals was also investigated up to 200 °C for 30 min. While Sn and Mo-based contacts performed just as well after annealing, $R_c$ of most other contacts increased. Te sublimation was a common source of thermal instability, with Te crystallites forming on the sides of contacts and within the gap.

### EM-ThP-25 RF Loss Improvement of GaN-HEMTs Grown on Silicon by Reduction of The Inversion Channel at Si Interface

***TienTung Luong***, *Y Chen, J You, S Chang, Y Ho, Y Lin,* National Chiao Tung University, Taiwan, Taiwan, Republic of China*; J Woo,* University of California, Los Angeles*; E Chang,* National Chiao Tung University, Taiwan, Taiwan, Republic of China

Regarding the unique characteristics (high breakdown field, high power density, high efficiency, and broadband) GaN are now broadly recognized as a key technology for many applications. In particular, GaN-based HEMTs are able to operate at high power, high frequencies, and high temperatures, exhibiting various excellent characteristics superior to those of conventional Si-based semiconductors. GaN-HEMTs on Si technology is expected to drastically reduce the fabrication cost. However, one of the main issues is the parasitic loss that can adversely impact the RF device performances. A free-electron inversion channel, which is caused by the positive piezoelectric charge at the AlN/Si interface induced by the piezoelectric field in the tensile AlN grown on Si, plays a critical role in the RF losses. An adoption of a low-temperature AlN near Si interface induces an unintentionally carbon-doped layer acting as a negatively fixed charge layer that is able to compensate for positive piezoelectric charge resulting in the improvements of both the RF losses and the leakage.

### EM-ThP-26 The Photoelastic Coefficient $P_{12}$ of $H^+$ Implanted GaAs as a Function of Defect Density

***Andrey Baydin***, *H Krzyzanowska, R Gatamov, N Tolk,* Vanderbilt University

The photoelastic phenomenon has been widely investigated as a fundamental elastooptical property of solids. This effect has been applied extensively to study stress distribution in lattice-mismatched semiconductor heterostructures. GaAs based optoelectronic devices (e.g. solar cells, modulators, detectors, and diodes) widely used in space probes are subject to damage arising from energetic proton $H^+$ irradiation. For that reason, the effect of proton irradiation on photoelastic coefficients of GaAs is of primary importance to space applied optoelectronics. However, there yet remains a lack of systematic studies of energetic proton induced changes in the photoelastic properties of bulk GaAs. In this work, the $H^+$ energy and fluence chosen for GaAs implantation are similar to that of protons originating from the radiation belts and solar flares. We present the depth-dependent photoelastic coefficient $P_{12}$ profile in non-annealed $H^+$ implanted GaAs obtained from the analysis of the time-domain Brillouin scattering spectra. The depth-dependent profiles are found to be broader than the defect distribution profiles predicted by Monte Carlo simulations. This fact indicates that the changes in photoelastic coefficient $P_{12}$ depend nonlinearly on the defect concentrations created by the hydrogen implantation. These studies provide insight into the spatial extent to which defects influence photoelastic properties of GaAs.

### EM-ThP-27 Manipulation of Elliptical Polarization and Modulation of Optical Activity using Terahertz Stereo-metamaterial Reflectors

***Elizabeth Philip***, *S Pal, S Stephens, P Kung, S Kim,* The University of Alabama

Metamaterials (MMs) are playing a vital role in the development of the field of photonics. These are artificial materials made by repeated arrays of meta-atoms of subwavelength size, and can be controlled to manipulate the electromagnetic (EM) waves interacting with them. With appropriate designing of these meta-atoms, it is possible to achieve unique EM properties such as perfect absorption, negative permittivity, negative permeability, electromechanically induced transparency, etc. Recently, in terahertz (THz) frequency regime, MMs are being employed to replace conventional polarization converters. Conventional polarizers, retarders, rotators, etc. are usually made using dichroic crystals and optical gratings that are bulky, less efficient and operate in narrow bandwidths. Whereas with MMs they can be made thin, compact, easily combinable and even flexible. Much of the current THz polarization converters made of MMs function only in the transmission mode [1]. Though there are a few that function in the reflection mode, these are mostly linear polarization converters [2]. Evidently, there is a lack of linear to elliptical or circular reflective polarizers in the THz regime. In this work, we take advantage of an interesting category of MMs called stereo-metamaterials (SMMs) to develop a linear to elliptical polarization converter. SMMs utilize the same meta-atom, but are arranged at different spatial positions. They are analogous to stereo-isomers, which are molecules constituting of the same atoms but have different spatial arrangements. Six separate devices with varying spatial arrangements are first optimized through simulations with finite element method using Comsol. By tailoring the spatial arrangement of the meta-atom, we manipulate the polarization of the reflected light to become elliptically polarized, achieving a maximum ellipticity angle of 20.5° at 0.240 THz. Furthermore, we modulate the optical activity of the device, and a pure optical rotation of 37.0° at 0.246 THz is attained from the simulation results. The devices are fabricated using standard photolithography techniques and their linear to elliptical polarization conversion and optical activity is successfully verified through THz ellipsometry measurements. The device sensitivity to incident polarization modulation and its corresponding reflective phase retardation response is also analyzed. Lastly, the influence of the dipole coupling and current distribution is studied in order to explain the microscopic origin for the manipulation of the reflected light. Such SMM with linear to elliptical polarization conversion and optical activity modulation properties in the reflection mode has promising applications in THz sensing and communication devices. [1] J.W. He, Z.W. Xie, S. Wang, X.K. Wang, Q. Kan, Y. Zhang, Journal of Optics. 2015;17(10):8. [2] N.K. Grady, J.E. Heyes, D.R. Chowdhury, Y. Zeng, M.T. Reiten, A.K. Azad, et al. Science. 2013;340(6138):1304-7.

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