

Monday Morning, October 28, 2013

Manufacturing Science and Technology

Room: 202 B - Session MS+AS+EM+EN+NS+TF-MoM

IPF 2013-Manufacturing Challenges: R&D Perspective (8:20-9:40 am) / Energy Storage (9:40 am-12:00 pm)

Moderator: K. Amm, GE Global Research, B.R. Rogers, Vanderbilt University

8:20am **MS+AS+EM+EN+NS+TF-MoM1 From Quanta to the Continuum: Opportunities for Mesoscale Science, G. Crabtree**, Argonne National Laboratory **INVITED**

Mesoscale science embraces the regime where atomic granularity and quantization of energy yield to continuous matter and energy, where high levels of complexity and functionality emerge from simple components, and where disparate degrees of freedom interact to produce entirely new behavior. Mesoscale science builds on the ever-growing foundation of nanoscale tools and insights that the community has developed over the last decade and continues to develop. Control of mesoscale complexity offers new scientific and technological opportunities: applying our mastery of nanoscale interactions to discover and design new architectures from the “bottom up” that display innovative macroscopic behavior and functionality. This constructionist approach to designing and building new functional architectures creates new horizons for mesoscale manufacturing, where principles of design and implementation differ fundamentally from conventional “top down” macroscopic approaches. Examples of mesoscale successes, challenges and opportunities will be described.

A more complete discussion of mesoscale science can be found in the BESAC report, *From Quanta to the Continuum: Opportunities for Mesoscale Science*, <http://science.energy.gov/bes/news-and-resources/reports/basic-research-needs/>

Innovative community input on opportunities for mesoscale science can be found on the *Mesosopic Materials and Chemistry* website, <http://www.meso2012.com/>

9:00am **MS+AS+EM+EN+NS+TF-MoM3 The National Network for Manufacturing Innovation – Towards a New Innovation Ecosystem for Advanced Manufacturing, M. Molnar**, National Institute of Standards and Technology **INVITED**

A key challenge to restoring U.S. leadership in advanced manufacturing is addressing the so-called “missing middle” – the technical and business barriers of scaling-up an innovative new material, process, or technology for robust production use. This plenary talk explores the National Network for Manufacturing Innovation as a means to accelerate U.S. innovation. As proposed by President Obama NNMI is a network of manufacturing institutes where Industry and Academia partner on industry-relevant challenges. Each institute would be chartered in a competitively selected topic and focus on nationally important, precompetitive technologies to create “innovation hubs” for transformational impact.

This plenary will review the NNMI progress to date, including the current design of the institute and supporting network and core functions. The emerging design builds on the extensive public input and the progress of the pilot institute on Additive Manufacturing, explored in detail in the following plenary. The discussion concludes with a review of the three manufacturing institutes topics being established this year.

9:40am **MS+AS+EM+EN+NS+TF-MoM5 Conformal Thin Films- The Use of Atomic Layer Deposition in Energy Related Applications, G.M. Sundaram**, Ultratech/Cambridge NanoTech **INVITED**

Atomic Layer Deposition (ALD) is a unique thin film deposition technique based on sequential precursor usage with self-limiting reactions, which yields films with excellent uniformity, density, conformality, and interface quality. This in turn has set the stage for its use in a wide array of technology areas. In this work, the principles of ALD will be covered, along with an examination of the intersection points between ALD and a number energy related structures - including storage devices.

10:40am **MS+AS+EM+EN+NS+TF-MoM8 Manufacturing a Three-dimensional, Solid-state Rechargeable Battery, A. Prieto**, Colorado State University, D. Johnson, Prieto Battery, Inc. **INVITED**

There are two main limitations to the rate of charging for Li-ion batteries: slow diffusion of Li⁺ into the electrodes and slow diffusion *between* them. The synthesis of high surface area electrodes has been shown to dramatically enhance performance because reducing the particle size of the

electrode material reduces the distance the Li⁺ ions have to diffuse. *The problem of decreasing the Li⁺ diffusion length between electrodes has not yet been solved.* We are working to incorporate high surface area foams of a novel anode material into a new battery architecture wherein the foam is conformally coated with an electrolyte made by electrochemical deposition, then surrounded by the cathode electrode. The significant advantage to this geometry is that the diffusion length for Li⁺ between the cathode and anode will be dramatically reduced, which should lead to much faster charging rates. However, if this battery is going to be useful and commercializable, it must be manufactured using low cost, reliable, scalable methods. I will present preliminary results on the initial stages of the battery architecture, including the fabrication of anode foams conformally coated with a polymer electrolyte. The reversibility of the intercalation into the anode and the ionic conductivity of the polymer electrolyte will be discussed.

11:20am **MS+AS+EM+EN+NS+TF-MoM10 Defects, Nonuniformities, and Degradation Mechanisms in Batteries, S. Harris**, Lawrence Berkeley National Laboratory **INVITED**

We review work from our laboratory that suggests to us that most Li-ion battery failure can be ascribed to the presence of nano- and microscale inhomogeneities that interact at the mesoscale, as is the case with almost every material; and that these inhomogeneities act by hindering Li transport. (Li does not get to the right place at the right time.) For this purpose, we define inhomogeneities as regions with sharply varying properties—which includes interfaces—whether present by “accident” or design. We have used digital image correlation, X-Ray tomography, FIB-SEM serial sectioning, and isotope tracer techniques with TOF-SIMS to observe and quantify these inhomogeneities. We propose new research approaches to make more durable, high energy density lithium ion batteries.

Monday Afternoon, October 28, 2013

Manufacturing Science and Technology

Room: 202 B - Session MS+AS+EM+NS+PS+TF-MoA

IPF 2013-Manufacturing Challenges for Emerging Technologies: III. Manufacturing Challenges: Electronics

Moderator: D. Seiler, National Institute of Standards and Technology (NIST), J. Hollenhorst, Agilent Technologies

2:00pm **MS+AS+EM+NS+PS+TF-MoA1 Graphene Materials and Devices Roadmap, L. Colombo, Texas Instruments** **INVITED**

The advancement of graphene and graphene based products will require a research and development progression similar to materials and development programs are now in full production, e.g. Si industry. The graphene research community has made significant progress over the past nearly a decade now in the physics and chemistry of graphene. We are now full engaged in the materials and device development and in some cases initial product stages. The introduction of any graphene based product will require the identification of materials, device and product metrics in order to properly keep track of the progress toward the product goals. In this presentation I will review and discuss the roadmap for various graphene based applications and present the status of materials and devices for nanoelectronic applications.

2:40pm **MS+AS+EM+NS+PS+TF-MoA3 Devices and Materials for the Post CMOS Area - What Are We Looking For?, W. Haensch, IBM T.J. Watson Research Center** **INVITED**

The long predicted end of scaling is coming. Many times it was predicted that the IC industry will hit a brick wall. Beginning in the early 1980's when patterning solutions were doomed to fail, then through the late 1990's when gate oxide scaling was thought to be at its end, and now in the recent years when device performance is thought to hit its physical limits. The truth is however that none of these posed an obstacle that could not be addressed. The reason while the progress of the industry enjoyed in the last several decades is slowing down is related to the ever increased power consumed to achieve ever higher performance. Seeing the end approaching, the quest for what is coming next is on! In this presentation I will give short review how we got where we are and what are the wonderful properties of MOSFET devices that allowed this extraordinary development. I will then look at the possibilities of a possible extension of the existing core logic technology. Finally I will discuss some alternate device options and provide a critical evaluation how they might fit into the IT landscape.

3:40pm **MS+AS+EM+NS+PS+TF-MoA6 Manufacturing Challenges of Directed Self-Assembly, R. Gronheid, IMEC, Belgium, P.A. Rincon Delgado, University of Chicago, T.R. Younkin, Intel Corporation, B.T. Chan, L. Van Look, I. Pollentier, IMEC, Belgium, P.F. Nealey, University of Chicago** **INVITED**

Directed Self-Assembly (DSA) of block copolymers (BCP) is based on nano-scale phase separation. Depending on the relative volume fraction of the blocks, different morphological structures may form in the bulk of these materials. In the case of di-block copolymers, specifically the lamellar and cylindrical phase provide structures that may be used to form line/space and hole-type patterns, respectively. When thin films of BCPs are applied on substrates that provide a pre-pattern to guide the assembly process, the orientation and direction of the resulting structures can be controlled. DSA has gained significant attention as a next method for mainstream nanofabrication in a time span of just a few years. The primary interest in the DSA technology includes the inherent variability control (since dimension is controlled through the polymer molecular weight) and the high pattern densities (typical length scales are on the order of 3-50nm) that are accessible. The outstanding questions that need to be answered in order to prove readiness of DSA for semiconductor manufacturing include defectivity, pattern transfer capabilities, pattern placement accuracy, design rule restrictions that are imposed by DSA and demonstration in an electrically functional device.

At imec, DSA based patterning has been implemented on 300mm wafers in various process flows that are compatible with semi-conductor manufacturing. These flows have been used as test vehicles to study the above-mentioned issues. In this paper, an overview will be given of the main recent accomplishments from the imec DSA program.

4:20pm **MS+AS+EM+NS+PS+TF-MoA8 Phase Change Memory, R. Bez, Micron, Italy** **INVITED**

Phase Change Memory (PCM) is a Non-Volatile Memory (NVM) technology that provides a set of features interesting for new applications, combining features of NVM and DRAM. PCM is at the same time a sustaining and a disruptive technology. From application point of view, PCM can be exploited by all the memory systems, especially the ones resulting from the convergence of consumer, computer and communication electronics. PCM technology relies on the ability of chalcogenide alloys, typically $\text{Ge}_2\text{Sb}_2\text{Te}_5$ (GST), to reversibly switch from amorphous state to poly-crystalline state. The two stable states differs for electrical resistivity, thus the information is stored in the resistance of the bit.

The alteration of the bit is possible thanks to melt-quench of the active material achieved by fast (10-100ns) electrical pulses. The energy delivered to program a bit is in the order of 10pJ, with a state of the art access time of 85ns, read throughput 266MB/s and write throughput 9MB/s. These peculiar features combined with data retention, single bit alterability, execution in place and good cycling performance enables traditional NVM utilizations but also already opened applications in LPDDR filed. Moreover PCM is considered the essential ingredient to push to the market the so called Storage-Class Memory (SCM), a non-volatile solid-state memory technology that is capable of fill the gap between CPU and disks.

In this perspective PCM technology can be effectively exploited in wireless systems, in solid state storage subsystem, in PCIe-attached storage arrays and in computing platform, exploiting the non-volatility to reduce the power consumption.

In order to be able to enter into a well established memory market there are key factors that must be fulfilled: i) match the cost of the existing technology in terms of cell size and process complexity, ii) find application opportunities optimizing the overall "memory system" and iii) provide a good perspective in terms of scalability. Phase Change Memory has been able so far to progress in line with all these requirements. Aim of this presentation is to review the PCM technology status and to discuss specific opportunities for PCM to enter in the broad memory market.

5:00pm **MS+AS+EM+NS+PS+TF-MoA10 450 mm Project, P. Farrar, University at Albany-SUNY** **INVITED**

The talk will focus on the leadership role the G450C consortium in driving the industry transition from 300mm to 450mm wafers. The current Status of the work at CNSE will be explored as well as the key role this public private partnership play is developing the process capability Required for High Volume Manufacturing. In addition critical success factors, and the ability to manage in a collaborative manner will be focused on.

Tuesday Morning, October 29, 2013

Manufacturing Science and Technology

Room: 202 B - Session MS+AS+BA+BI+PS+TF-TuM

IPF 2013-Manufacturing Challenges for Emerging Technologies: IV. Manufacturing Challenges: The Life Sciences

Moderator: D.G. Castner, University of Washington, L.J. Gamble, University of Washington

8:00am **MS+AS+BA+BI+PS+TF-TuM1 Microfluidics for Chemical Analysis**, L. Carr, Q. Bai, R. Brennen, S. Post, G. Staples, K. Seaward, H. Yin, L. Martinez, D. Ritchey, K. Killeen, Agilent Technologies **INVITED**

Chemical analysis is an essential tool for pharmaceuticals, environmental testing, food safety, forensics, energy and many other industries. The need for faster, more accurate and more sensitive measurements continuously pushes the limits of measurement technology and creates opportunities for advances in chemical analysis instruments and applications. One way in which this need can be addressed is by incorporating microfluidic devices in High Pressure Liquid Chromatography (HPLC). Pressure-based microfluidic chips have enabled a new class of reproducible integrated workflow devices that combine sample preparation, enrichment, and HPLC separation *with an integrated ESI/MS (Electrospray Ionization/Mass Spectrometry) interface* for high sensitivity nanoflow Liquid Chromatography-Mass Spectrometry (LC-MS). These devices have most commonly been fabricated using polymer, ceramic, and glass materials but the next generation of higher capacity and throughput microfluidic chips for LC-MS requires materials and structures capable of ultra high pressure operation. In this work, we describe the fabrication and performance of diffusion-bonded metal chips for high performance nano- and microflow LC-MS operation. The microfabrication technology required to make these devices includes semiconductor fabrication standards such as photolithography and thin film deposition, as well as laser ablation, electrochemical etching, and diffusion bonding. These novel metal devices exhibit state of the art performance in resolution and throughput for microfluidic LC-MS chips. These chips are an example of improvements in measurement sensitivity, resolution, speed, and ease of use that have been made possible by utilizing microfluidic devices for chemical analysis.

8:40am **MS+AS+BA+BI+PS+TF-TuM3 Challenges in the Fabrication of Nanoscale Devices for DNA Base Sensing**, S. Papa Rao, J. Bai, E.A. Joseph, R.L. Bruce, M. Lofaro, M. Krishnan, M. Brink, M. Guillorn, S.M. Rossmagel, Q. Lin, J. Cotte, C. Jahnes, Smith, Gignac, Reuter, Nam, Astier, Wang, Stolovitsky, Goldblatt, IBM Research Division, T.J. Watson Research Center **INVITED**

The fabrication of integrated circuits with increasingly fine geometries has required the development of advanced process technologies, which can be further refined for the purpose of building devices for biological applications. Applications such as sensing nucleotides in DNA require structures that are of the order of a few nanometers. This talk will focus on the specific challenges encountered in the fabrication of such nano-scale devices – broadly classified into materials-related challenges, unit-process challenges and process integration-related challenges. Issues such as dielectric integrity, metal recrystallization, and materials compatibility with chemistries used down-stream will be discussed. Dimension control during fabrication of ~10 nm sized structures was achieved through intense process development efforts of reactive ion etch and chemical mechanical planarization (both manufacturing-friendly techniques). Device layout issues that affect manufacturability will be presented. Finally, some of the important lessons learned in achieving a high yield of reliable devices through process-integration changes will also be discussed.

9:20am **MS+AS+BA+BI+PS+TF-TuM5 Nucleic Acid Synthesis and Applications**, S. Laderman, Agilent Technologies **INVITED**

The pursuit of perfect and practical *de novo* chemical syntheses of nucleic acids has been the foundation of a broad range of life science accomplishments over many decades in the past. Its further pursuit is enabling a broad range of opportunities many decades into the future. These themes will be elucidated by examining the precedents and improvements enabling high throughput genomics for research and diagnostics through the manufacturing of high quality DNA microarrays and complex pools of long oligonucleotides. Looking forward, new ways to synthesize RNA will enable deeper understanding and improved manipulations of cells, tissues and organisms. At the same time, multiple applications of synthetic biology

are motivating additional focus on further advances in flexibly and cost-effectively constructing perfect DNA.

10:40am **MS+AS+BA+BI+PS+TF-TuM9 Single Molecule, Real-Time DNA Sequencing**, S. Turner, Pacific Biosciences **INVITED**

In this talk, I'll convey the story of the development and commercialization of Pacific Biosciences' Single Molecule, Real-Time DNA Sequencing technology. I will start with an overview of the method, how it works, and how it differs from sequencing methods that came before it. I will continue with a discussion of some key technology milestones, with an emphasis on the technological advances in materials engineering and nanofabrication. I'll finish by showing some examples of how this technology has transformed the field of DNA sequencing and genome analysis.

11:20am **MS+AS+BA+BI+PS+TF-TuM11 Opportunities and Challenges in the Biobased Products Manufacturing**, J. Flatt, S. Bailey, S. Bower, D. Gibson, S. Farah, J. Butler, J. Hannon, Synthetic Genomics **INVITED**

Biobased production of life's necessities, including food, fuels, chemicals and medicines provides a foundation for sustainable and geographically distributed manufacturing processes. Biobased manufacturing utilizes photosynthetic processes directly through conversion of carbon dioxide and light energy or indirectly through conversion of renewable biomass feedstocks to products. Biological cells (biocatalysts) are the operating systems for these biobased manufacturing processes. Rapid advances in synthetic biology enable the engineering of biocatalysts which can produce a broader range of products than previously possible, at high yields and productivities necessary for achievement of desired economics. Improvements in biocatalysts are achieved through modifications of DNA, which is the software of living systems. Significant advances in the costs, fidelity and speed of DNA synthesis, along with improving understanding of gene function and regulation is enabling the more rapid development of biocatalysts which achieve required performance for commercially viable manufacturing processes. The current state of the art of synthetic biology and technology trends which will impact future development of biobased processes will be discussed. Additional market-specific and process-specific challenges exist, and will be discussed in context of the specific examples taken from manufacture of synthetic vaccines, biobased chemicals and fuels. Recently, Novartis and Synthetic Genomics demonstrated the ability to successfully produce vaccines for prevention of seasonal influenza using synthetic DNA constructs, which significantly reduces the time from influenza strain identification to production of the vaccine seed. Development of this revolutionary process required significant improvement of the fidelity of DNA synthesis and assembly, which provides insight into the challenge of engineering more complex biocatalysts. On the other end of the spectrum, phototrophic microalgae have great long-term potential to provide a sustainable and alternative source of food and liquid transportation fuels. Phototrophic microalgae can be cultivated using non-potable water on non-arable land. Techno-economic analysis (TEA) and life cycle assessment (LCA) both suggest that significant improvements in biocatalyst productivity and capital cost reduction will be required to achieve competitive economics. Maximum observed algal biomass productivities in the range of 20 to 25 g/m²/day are far lower than generally-agreed upon theoretically-achievable productivities based upon the actual solar energy available. Improvement of photosynthetic efficiency in mass culture is required for economical algal-based processes. Limited availability of light in mass culture also limits the maximum achievable cell density, which results in increased downstream processing costs. The challenges of "dilute solution economics" associated with commercial algae production and potential biological and engineering solutions will be discussed.

Tuesday Afternoon, October 29, 2013

Manufacturing Science and Technology

Room: 202 B - Session MS+AS+EL+EM+PS+TF-TuA

Manufacturing Challenges of Nanoscale Patterning

Moderator: E.B. Svedberg, The National Academies

2:00pm **MS+AS+EL+EM+PS+TF-TuA1 Alphabet-Based Template Design Rules - A Key Enabler for a Manufacturable DSA Technology.** *H. Yi, H.-S.P. Wong*, Stanford University **INVITED**

Block copolymer DSA is a result of spontaneous microphase separation of block copolymer films, forming periodic microdomains including cylinders, spheres, and lamellae. Among all the various self-assembled structures, cylinder patterns have attracted specific interest due to their great potential in patterning electrical contacts in Integrated Circuits (ICs). Due to the random distribution of electrical contacts in layouts as well as the continuous scaling of IC circuits, patterning contacts has become increasingly challenging for traditional optical lithography. Due to the advantage of low cost and sub-20 nm feature sizes, block copolymer directed self-assembly (DSA) is a promising candidate for next generation device fabrication.

Traditionally, the study of DSA has been focused on achieving long range order and a periodic pattern in large area. Chemoepitaxy approaches including using chemical patterns of preferential affinity on the substrate surface or controlling pattern formations by tuning annealing conditions have been investigated and developed. They can improve the long range order self-assembly quality and lower the defect density over large areas. In order to use DSA to pattern the randomly distributed contacts in IC layouts, we adopt physical (topographical) templates to form irregularly distributed cylindrical patterns. Topographical templates use strong physical confinements in lateral directions to alter the natural symmetry of block copolymer and guide the formation of DSA patterns. Previously we have demonstrated that for the first time the self-assembled features can be almost arbitrarily placed as required by circuit fabrication and not limited to regular patterns, by combining templates of different types on one wafer. These various templates are akin to the letters of an alphabet and these letters can be composed to form the desired contact hole patterns for circuit layouts. The capability of arbitrary placement is demonstrated in industry-relevant circuits such as static-random-access-memory (SRAM) cells and standard logic gate libraries at a dimension that is the state-of-the-art semiconductor technology today [1]. To enable introduction of DSA into manufacturing we developed a general template design strategy that relates the DSA material properties to the target technology node requirements. This design strategy is experimentally demonstrated for DSA contact hole patterning for half adders at the 14 nm and 10 nm nodes [2].

Reference:

[1] H. Yi et al. *Adv. Mater.*, 2012.

[2] H. Yi et al. *SPIE*, 2013.

2:40pm **MS+AS+EL+EM+PS+TF-TuA3 Characterizing the Sensitivity of Block Copolymer Directed Self-Assembly Processes to Material and Process Variations.** *C. Henderson, A. Peters, R. Lawson, P. Ludovice*, Georgia Institute of Technology

Future scaling of integrated circuits (IC) is in jeopardy due to a number of challenges related to both future material and process requirements that are needed to allow for fabrication of sub-20 nm IC devices. One of the most critical challenges is that of developing patterning technologies that can allow for formation of sub-20 nm patterned structures in a fast and economically viable manner. Due to difficulties with alternative technologies, techniques that can extend the use of current 193 nm optical lithography in a cost effective manner would be very attractive. Directed Self-Assembly (DSA) using block copolymers to perform pitch subdivision of lithographically generated primary patterns is one such promising technology. In this technique, a lithographic method is first used to define a topographic or chemical template pattern on a surface. This surface is then coated with a block copolymer that is further processed to induce microphase separation. The presence of the topographic or chemical patterns on the surface aligns, registers, and provides long range order to the formed block copolymer patterns. This microphase separation-based patterning process utilizes the propensity of the block copolymer to naturally form nanometer scale patterns whose size are dictated by the polymer block molecular weight.

The overarching goal of our work has been to develop both new block copolymers that can enable sub-20nm DSA patterning and to develop the experimental and modeling tools needed to understand the limits of such

processes. In this paper, we will review our recent systematic studies of block copolymer DSA processes using state-of-the-art molecular dynamics simulations. The aim of these studies has been to identify the important material and process factors that affect the DSA process and to quantify the sensitivity of the DSA process to these factors. For example, the influence of polymer block molecular weight control and polydispersity on patterning have been rigorously quantified. Furthermore, processing factors such as guiding pattern mis-sizing and low level surface topography in the guiding pattern and their effect on DSA patterning have been studied in detail. Studies have also been performed via simulation using thermodynamic integration methods to calculate the free energy of defects in such DSA systems and the sensitivity of such defect free energies to important material and process parameters. We will review the outcomes of these studies to illustrate what the important material and process challenges will be in adapting block copolymer DSA methods into a manufacturable technology.

3:00pm **MS+AS+EL+EM+PS+TF-TuA4 DSA Patterning for sub-40 nm Pitch Features.** *I.C. Estrada-Raygoza, C. Liu, Y. Yin, J. Abdallah*, IBM Albany Nanotech Center, *S. Mignot*, GLOBALFOUNDRIES U.S. Inc., *B.G. Morris, M.E. Colburn*, IBM Albany Nanotech Center, *V. Rastogi, N. Mohanti, A. Raley, A. Ko*, TEL Technology Center, America, LLC

As the semiconductor industry targets sub-40 nm pitch features, there will be a necessity for new patterning techniques which allow for the extension beyond single ArF-immersion patterning capability of 38 half pitch features. To meet today's aggressive design requirements, double patterning techniques, such as Pitch Splitting (PS) Lithography and Sidewall Image Transfer (SIT), have been widely used. Below 38 nm pitch design the industry has looked toward Extreme Ultraviolet (EUV), Double Sidewall Image Transfer (SIT2) and Directed Self-Assembly (DSA) as strong emerging candidates. A major component to the success of the DSA technique is the development of effective etch processes. This talk targets to discuss the challenges and innovations of the plasma etch process on sub-40 nm pitch features produced by DSA chemo and grapho-epitaxy guiding patterns. Each DSA scheme presents different challenges, depending of the aspect ratio, density of the patterns and etch stack materials, but in general, the parameters that have been studied are selectivity to both masking and etched materials, across wafer profile uniformity, critical dimension (CD) uniformity and line-edge/line-width roughness (LER/LWR). This work was performed by the Research Alliance Teams at Albany IBM Research and Development Facilities.

4:40pm **MS+AS+EL+EM+PS+TF-TuA9 Advanced Gate Patterning Techniques for 14nm Node and Beyond.** *F.L. Lie, R. Jung, Y. Yin, A. Banik, S. Kanakasabapathy, J.C. Arnold, S. Seo, B. Haran*, IBM Corporation, *Y. Moon, L. Jang, S. Bentley*, GLOBALFOUNDRIES U.S. Inc., *H. Kang, D. Bae*, Samsung Electronics Co., *A. Metz, C. Cole, K. Ito, S. Voronin, A. Ko, A. Ranjan, K. Kumar*, TEL Technology Center, America, LLC

For advanced CMOS nodes, traditional patterning processes are challenged to meet the technology needs of certain key levels. For example, conventional 193nm immersion lithography is not able to resolve features below 40nm half pitch with a single exposure without severe design rule restrictions. Until further wavelength scaling through Extreme Ultraviolet (EUV) has matured, the industry's attention is focused on advanced patterning schemes such as Pitch Splitting (PS) Lithography and Sidewall Image Transfer (SIT). In PS, a pattern is defined by two lithography exposure with a certain coordinate shift between the two exposures. PS can be achieved through either litho-etch-litho-etch or litho-litho-etch. In SIT, a pattern is defined by creating a mandrel in one lithography exposure, depositing a conformal spacer film on the mandrel, and pulling out the mandrel, resulting in two standing spacer for the pattern frequency doubling. This work evaluated the advantages and technical challenges of PS and SIT patterning schemes for line-space application. We will focus on CD uniformity improvement, line edge/line width roughness control, pitch walk control, and the extendability of each technique. RIE challenges common to double patterning such as through pitch etch bias will also be discussed.

This work was performed by the Research Alliance Teams at various IBM Research and Development Facilities and in joint development with TEL Technology Center, America, LLC

5:00pm **MS+AS+EL+EM+PS+TF-TuA10 High Throughput Electrospinning of Ceramic Nanofibers.** *S. Sood, P. Gouma*, State University of New York at Stony Brook (Stony Brook University)

High yield nanomanufacturing has been the focus of greater attention due to the emerging importance of functional nanomaterials. Electrospinning is a

nanomanufacturing process that faces challenges as far as its scalability is concerned. Even the existing high-throughput electrospinning systems are limited to processing thin layers of polymer nanofibrous mats. Nanofibrous ceramics have rarely been studied with respect to their electrospinning processing. On the other hand, electrospun nanowires of ceramics are key to nanotechnology and nanomedicine applications (e.g. electrospun MoO₃ nanowires have been used as ammonia sensors for application in non-invasive diagnostics [1]). In this study, the scalable synthesis of ceramic oxide nanomats by the multi-jet design that we developed and built and which enables very high yield of ceramic nanofibers is discussed. As a scaled up approach to traditional needle electrospinning [2], up to 24 jets are spun simultaneously using similar processing parameters as a traditional needle set up. Due to a thin metallic disc design, with tiny holes drilled at the disc, the electric field is evenly distributed to all jets. Continuous replenishment of the source disk at higher flow rates allows for high yields of nanofibers.

P. Gouma, K. Kalyanasundaram, and A. Bishop, "Electrospun Single Crystal MoO₃ Nanowires for Bio-Chem sensing probes", *Journal of Materials Research, Nanowires and Nanotubes special issue*, 21(11), pp. 2904-2910, 2006.

S. Sood, S. Divya, P. Gouma, "High throughput electrospinning of 3D nanofibrous mats". *Journal of Nanoengineering and Nanomanufacturing*. Accepted Publication. In Print, 2013.

5:20pm **MS+AS+EL+EM+PS+TF-TuA11** **Manufacture and Characterization of Silver and Copper Nanorods Produced via Forcespun Nylon 6 Nanofibers Templates**, *D.M. Mihut, K. Lozano, W. Zhao*, The University of Texas Pan American

The Nylon 6 nanofibers are produced using the forcespinning method and further on coated with metallic thin films using the thermal evaporation equipment. The Nylon 6 nanofibers are used as templates in order to obtain silver and copper nanorods where the polymer is removed after high temperature calcination from the metallic coated structures. The metallic nanorods morphology and electrical behavior are characterized using the scanning electron microscopy, scanning transmission electron microscopy (SEM, STEM), energy disperssive X-ray spectroscopy (EDX) and electrical measurements. This method of fabrication offers the ability to obtain controlled ultrafine size netallic nanorods.

Tuesday Afternoon Poster Sessions

Manufacturing Science and Technology

Room: Hall B - Session MS-TuP

Aspects of Manufacturing Science and Technology Poster Session

MS-TuP2 Investigation on Environment Concerns of Scanning Electron Microscopy (SEM) for Nanomanufacturing Application. *F.C. Hsieh, P.H. Lin, C.Y. Huang, N. Chu, J.S. Kao*, National Applied Research Laboratories, Tawain, Republic of China

Scanning electron microscopy (SEM) is used for surface morphology measurement of thin films in nanomanufacturing such as: atomic layer deposition (ALD), nanosphere lithography, and nanoimprint et al. For those nanomanufacturing applications, the surface morphology of thin films could affect the desired properties. As a result, the quality of the image of surface morphology must be evaluated. In this study, the effects of microwave intensity and vibration frequency are investigated. For accelerating voltage of 15kV at magnification of 150,000, the microwave intensity of alternative current (ac) of electric equipment must below 90nT. However, at 15kV accelerating voltage and 50,000 magnifications, the microwave intensity of ac must below 70nT. Besides, the allowable amplitude increases with vibration frequency between 2Hz and 5Hz. The maximum amplitude was 6.0 μ m (peak to peak) at 5Hz of vibration frequency. The proposed investigation can provide a suggestion to ensure the accuracy and stability of measurement for SEM.

Wednesday Morning, October 30, 2013

Accelerating Materials Discovery for Global Competitiveness Focus Topic

Room: 202 B - Session MG+EM+MI+MS-WeM

Materials Discovery and Optimization through Iterative Approaches

Moderator: M.B. Holcomb, West Virginia University, S. Jones, National Science Foundation

8:40am **MG+EM+MI+MS-WeM3 Preparation of Ultra Stable Organic Glasses by Physical Vapor Deposition, J.J. de Pablo**, University of Chicago, *L. Yu, M.D. Ediger*, University of Wisconsin-Madison **INVITED**

There is considerable interest in identifying structure-property relations in glasses. Structural studies of glassy materials have benefited from insights provided by molecular simulations of model glass forming liquids. In particular, simulations have provided support for the existence of dynamic and mechanical heterogeneity at the level of small groups of molecules or particles. In general, however, the cooling rates employed in simulations have been many orders of magnitude faster than in experiments, thereby adding some level of ambiguity to direct comparisons between theory and experiment. Recently, experiments have shown that glasses of organic molecules having unusually large thermal and kinetic stability can be prepared by a vapor deposition process. Such glasses exhibit higher onset temperatures, higher densities, and higher mechanical constants than those of ordinary glasses. In particular, vapor-deposited glasses have been shown to exhibit relaxation times that are many orders of magnitude longer than those of ordinary glasses. Inspired by such experiments, we have devised a strategy that allows one to prepare highly stable glassy materials, in silico, having thermal and kinetic characteristics that are superior to those obtained by gradual cooling of liquid samples. In this presentation, we will describe current experimental efforts to produce and characterize stable glasses, along with an overview of available theoretical and computational strategies aimed at understanding their properties. Emphasis will be placed on recent attempts to identify the structural origins behind the extraordinary stability of vapor deposited glasses, with the goal of providing new insights for design of stable amorphous materials deep in the potential energy landscape.

9:20am **MG+EM+MI+MS-WeM5 Composition and Structure Manipulation for Energy Materials with Improved Properties, S. Lany, H. Peng**, National Renewable Energy Laboratory, *V. Stevanovic*, Colorado School of Mines

Ideally, materials for energy applications like photovoltaics, photo-electro catalysis, or thermoelectrics should have a high performance, but be earth-abundant and manufacturable by low-cost processes. Given such demanding constraints, the list of promising materials that could potentially fulfill all requirements often shrinks to a few hopefuls. Then, the question arises whether we can start from materials that have both good and bad features, and manipulate the composition and structure such to cure their deficiencies. The role of theory is to assess the properties and identify promising alloying approaches.

We are presenting two recent examples for this approach: As a photovoltaic material, Cu₂O suffers from a high absorption threshold due to a relatively large band gap and a forbidden optical transition. Also, the p-type doping is 1-2 orders of magnitude below the optimal level. Our theoretical work identifies alloying of Zn, S and Se as a promising route to improve the optical and electrical properties of Cu₂O. Strong dopant-defect interactions lead to the unusual situation that the isovalent (S, Se) alloying increases the electrical doping, whereas the aliovalent (Zn) alloying changes the optical properties. The second example of MnO-ZnO alloys is based on the prediction [Phys. Rev. B 85, 201202(R) (2012)] that MnO in a hypothetical tetrahedral structure (zinc-blende or wurtzite) should have a smaller band gap and superior carrier transport properties than the normal octahedral rocksalt structure. These features would make this hypothetical material interesting, e.g., for photo-electro-catalytic water-splitting. We predict that Mn_{1-x}Zn_xO alloys assume the wurtzite structure above x = 0.38, and that such alloys preserve the beneficial properties of the tetrahedral MnO phase. Thus, the alloy approach presents a viable path to realize desirable materials properties that were originally identified for a hypothetical material.

9:40am **MG+EM+MI+MS-WeM6 Accelerated Optimization of Solar Cell Materials, A. Zakutayev**, National Renewable Energy Laboratory, *V. Stevanovic*, Colorado School of Mines, *S. Lany, J. Perkins, D. Ginley*, National Renewable Energy Laboratory

The rate of progress in the field of solar cells has been historically limited by the need for materials with desired functionality. Two complementary high-throughput approaches that have potential to facilitate such innovation are combinatorial thin-film experiments and predictive first-principles theory. Here we present examples of accelerated optimization of solar cell materials using the combined theoretical/experimental approach. The specific examples include (i) photovoltaic absorbers, and (ii) p-type contacts for solar cells

(i) PV absorbers are the key elements in any solar cells. Functionally, the absorbers are required to (1) absorb sunlight, and (2) facilitate extraction of charge carriers. We demonstrate accelerated progress towards (a) enhancement of optical absorption in Cu₂O, (b) improvement of electrical charge transport properties of Cu₃N, and (c) optimization of Cu-Sn-S material with respect to both optical and electrical properties. Our progress towards integration of these materials into thin film solar cell prototypes also will be discussed.

(ii) p-type contacts are needed for next-generation thin-film photovoltaics. Functionally such p-type contacts are required to (1) transmit sunlight, and (2) conduct holes. To accelerate the progress, we show (a) formulation of design principles (d₆ oxide spinels) to guide the candidate selection [1, 2, 3], (b) down-selection of the most promising materials (Co₂ZnO₄ and Co₂NiO₄) from ~30 candidates using predictive theory [4], (c) optimization of the selected best-of-class materials (Co-Zn-O, Co-Ni-O) using thin-film combinatorial experiments [5], and (d) integration of the optimized materials (Zn-Ni-Co-O) as hole transport layers in organic photovoltaic devices [6].

In summary, combination of high-throughput theoretical and experimental methods demonstrated here can significantly accelerate the development of materials for thin film solar cells. This approach should be also suitable for discovery and optimization of materials for other technological applications.

This research is supported by U.S. Department of Energy, as a part of two NextGen Sunshot projects, an Energy Frontier Research Center, and a "Rapid Development" agreement.

[1] V. Stevanovic et al Phys. Rev. Lett. 105, 075501 (2010)

[2] V. Stevanovic et al J. Am. Chem Soc. 133, 11649 (2011)

[3] J. Perkins, A. Zakutayev et al Phys. Rev. B 84, 205207 (2011)

[4] T. Paudel, A. Zakutayev et al Adv. Func. Mat. 21, 4493 (2011)

[5] A. Zakutayev et al Phys. Rev. B 85, 085204 (2012)

[6] A. Zakutayev et al MRS Comm. 1, 23 (2011)

10:40am **MG+EM+MI+MS-WeM9 The "Materials Genome" Project: Accelerated and Large-Scale Materials Discovery through Computation, G. Ceder**, MIT **INVITED**

Novel materials design has become a critical capability to address several urgent societal problems. The need for novel materials is the technological Achilles Heel of our strategy to address the energy and climate problem facing the world, and over-reliance on critical elements has inspired large efforts to develop accelerated materials design strategies. The Materials Genome Project, originally started at MIT (www.materialsproject.com), has as its objective to use high-throughput first principles computations on an unparalleled scale to provide basic materials property data on all known and many potential new inorganic compounds, thereby facilitating the search for new materials.

I will show successful examples of high-throughput calculations in the field of lithium battery, and show several new materials that have been discovered. I will discuss the public release version of the Materials Genome project which is making large quantities of computed data freely available to the materials community. The Materials Project is rapidly growing as a large collaborative environment for computed materials data.

11:20am **MG+EM+MI+MS-WeM11 Multifunctional Interfacial Materials by Design, C. Eom**, University of Wisconsin-Madison **INVITED**

Complex oxides materials have been fertile ground for new discoveries, due particularly to their wide-ranging electronic, optical, and magnetic properties. Interfaces between complex oxides and related materials create juxtapositions between different symmetries and ordered states, and it has become clear that these interfaces are new materials in their own right and lead to dramatically different properties from those in bulk. But interfacial materials encompass a virtually unexplored territory, one in which theory or

experiment alone cannot be successful. New approaches must be implemented to understand basic principles, categorize competing interactions, and design and synthesize complex oxide interfaces with advanced functionalities. Our project focuses on an iterative cooperation between forefront theory and experiment that determines the fundamental principles controlling new physical phenomena at oxide interfaces, uses these principles to design couplings between multiple orders at interfaces to generate new functionalities, and experimentally synthesizes and investigates designed interfacial materials for novel electronic devices. These atomic-scale interfacial materials lead to, for example, new classes of electric-field controllable electronic and magnetic phenomena, and enable the development of new technologically important devices that exploit these couplings. Using a predictive theory and modeling, and feedback to theory from experiments, we have designed and synthesized novel oxide hetero-interfaces that have unique properties not presently available. This work has been done in collaboration with M.S. Rzchowski, C.J. Fennie, E.Y. Tsybal, L.Q. Chen, X.Q. Pan, S. Ryu, T. Hernandez, T. R. Paudel, H. Zhou and D. D. Fong.

Wednesday Afternoon, October 30, 2013

Accelerating Materials Discovery for Global Competitiveness Focus Topic
Room: 202 B - Session MG+EN+MS-WeA

Education for Interactive R&D & Industrial Implementation

Moderator: C. Eom, University of Wisconsin-Madison, B. Nelson-Cheeseman, University of St. Thomas

2:00pm **MG+EN+MS-WeA1 21st Century Skills and Educating the Next Generation Workforce for Expedited Innovation and Deployment, C.C. Broadbridge**, Southern Connecticut State University **INVITED**

The goal of the Materials Genome Initiative [MGI] is to expedite materials discovery, innovation and deployment via the development of new approaches to materials research that exploit interdisciplinary collaboration and innovation. Successful implementation will require a workforce possessing 21st Century Skills including critical thinking, problem solving, communication, collaboration, technological fluency and creativity. To address the need for US competitiveness in a global economy, educational reform has been initiated at the K-12 level with the development of 21st Century Skills Standards [1], Common Core Standards [2] and the Next Generation Science Standards [3]. Similar reform is needed at the university and post-graduate [PG] professional development levels to assure the optimal development of a STEM educational pipeline. At the university level, reform has been initiated with the development of novel approaches to all university [non-major] requirements as well as courses and programs for majors (e.g., [4,5]). For the effective implementation of the MGI, it is important to realize the natural synergies that exist between these efforts and those within the materials science education and research communities. Arguably, individuals acquire and refine these necessary skills best via exposure to, and active participation in, authentic science research. NSF funded Materials Research Science and Engineering Centers [MRSECs] support interdisciplinary and multidisciplinary materials research and education of the highest quality [6]. All MRSECs include education and outreach components that effectively integrate the collaborative and innovative aspects of materials research. Components are developed and implemented at the K-PG levels and also include programs that educate the general public. For this presentation, educational reform at all levels will be reviewed with an emphasis on approaches with the greatest potential positive impact on the implementation of the MGI. In particular, an interdisciplinary team-based approach to materials research effectively leveraging programs within the Center for Research on Interface Structures and Phenomena (CRISP) MRSEC will be described that integrates materials science education and research while maximizing on the attainment of the 21st Century Skills necessary for successful implementation of the MGI.

1. <http://www.p21.org/overview/skills-framework/351>
2. <http://www.corestandards.org/>
3. <http://www.nextgenscience.org/>
4. <http://www.aacu.org/resources/generaleducation/index.cfm>
5. <http://www.tms.org/pubs/journals/jom/0910/thornton-0910.html>
6. <http://www.mrsec.org/>

2:40pm **MG+EN+MS-WeA3 High-Performance Ceramics – Challenges for Next Generations, W. Rossner, S. Lampenscherf**, Siemens AG, Germany **INVITED**

Ceramics play an important role in system engineering for demanding industrial applications because they provide functionality of key components that are critical for overall system performance and operational benefit. The continuous development of high performance ceramics over the last decades was aiming mainly towards 'better' properties and 'deeper' understanding of material behaviour.

For today's applications in areas such as power engineering, medicine, automotive, aircraft and high-end electronics the time-to-market aspect is an important success factor. Product cycles become shorter while R&D cycles especially including materials development are not able to keep up with such pace. The complex relationship between ceramic performance and processing plays a special role for accelerating the R&D process. An additional time-consuming factor is the need for extensive qualification and testing of high-performance ceramics to guarantee functionality and reliability under desired operation conditions.

Based on the very much improved understanding of the dependencies of processing, performance and application as well as the availability of

advanced computational methods and tools materials engineering can be a vital part to overcome today's limitations for accelerating materials development and product implementation.

In the talk we discuss these aspects in the context of current industrial examples for next generation high performance ceramics.

4:00pm **MG+EN+MS-WeA7 Educating for High-Impact Computation - Skills vs. Acceptance, W.E. Windl**, The Ohio State University **INVITED**

As an integral part of the Materials Genome Initiative (MGI), the task of materials computation, in concert with experiment and theory, is to help accelerate the discovery and maturation of new materials by at least a factor of two. During the first rounds of MGI-related solicitations, two major groups of challenges that always existed became very evident. For one, the obvious question about the skill set available in the Materials Research community to actually perform the necessary computations. Secondly, and much less apparent on the surface, was the frequent lack of acceptance of computational work as a valid input, maybe foremost in the experimental community, which can lead to awkward situations, missed opportunities, and frustration in collaborative projects. Beginning with the 2012-2013 academic year, The Ohio State University has moved from a quarters-based academic calendar to a semesters-based calendar. As part of this change, the Department of Materials Science and Engineering has elected to revise degree program curricula in a significant manner. A key objective in our revision was to respond to the challenges in lack of acceptance of computational work from Integrated Computational Materials Engineering and MGI described above. We have developed a curriculum that attempts to integrate congruently database use, visualization, simulation and computational approaches in materials science with other core educational content. At the undergraduate level, our goal was to produce graduates who are cognizant of the broad range of computational tools available to materials engineers and what they can do to solve engineering problems, and who are able to use a number of those tools proficiently to solve problems of practical importance themselves. The MSE core curriculum includes 9 credit hours (four courses), or 20% devoted to these topics. Students may take an additional 4 credit hours (two courses) in elective content on computational methods in materials science. In this presentation, details will be presented on the specific course offerings, course content, exercises, and software packages used. How the courses are postured in the curriculum will also be addressed. The experiences, challenges, and recommendations resulting from the first year of teaching will finally be discussed, where the author was involved in four different courses relying on different combinations of traditional teaching with reverse and peer teaching approaches as well as with significant fractions of active-learning work.

4:40pm **MG+EN+MS-WeA9 MGI in the Laboratory: Closing the Feedback Loop in Aerospace Materials Design and Development, E. Sapper, P. Kinlen**, Boeing Research & Technology **INVITED**

The aerospace industry has continuously driven major developments in material science as technology has evolved from wood and fabric to lightweight metal alloys and advanced polymer composites. Future aerospace materials systems will require even more advanced technologies, such as those afforded by smart and responsive systems like electroactive polymers and composites. The unique properties of these materials provide the ability to construct intelligent systems which produce a defined, predictable response to an input.

Concurrent with state-of-the-art chemical technology, the increasing availability of high-performance computing power has facilitated the entry of various computational simulation and modelling methods into the research and development production cycle. Quantum mechanics, molecular dynamics, and multi-scale simulation approaches, developed and applied within a Materials Genome Initiative paradigm, are providing insight into aerospace material properties of interest, such as species-specific transport rates, electrochemical response, service lifetime prediction, material color and appearance, and quantitative structure-property relationships.

The ultimate goal of a coupled experimental-computational approach is the closed and tightened feedback loop between laboratory results and computational predictions. This leads to the incorporation of more theory into experimental practice as well as more heuristics into computational method development, expressed in the form of semi-empirical models and empirically-pinned property response surfaces. This presentation will review some of the challenges involved in applying advanced computational methods alongside state-of-the-art laboratory procedures. The development of novel, more environmentally friendly aerospace coatings that release site-specific corrosion inhibitors on-demand will be presented as a case-study in closed-loop computation-experimentation.

5:20pm **MG+EN+MS-WeA11 Condensed Matter Physics in an Age of Computation**, *M. Marder*, University of Texas at Austin **INVITED**

Condensed matter physics and materials physics have grown so enormously that no one can hope to know everything done in the last five years let alone the last fifty. This does not relieve researchers of the charge of educating new generations of students. I will discuss the balance between acquisition of skills and acquisition of knowledge, and the way that computing power changes what is taught and how.

Friday Morning, November 1, 2013

Graphene and Other 2D Materials Focus Topic

Room: 101 A - Session GR+EM+MS+NS+SP-FrM

2D Materials: Device Physics & Applications

Moderator: L. Cao, North Carolina State University, E.

Riedo, Georgia Institute of Technology

8:20am GR+EM+MS+NS+SP-FrM1 Epitaxial Graphene Electronics, **J.A. Robinson**, The Pennsylvania State University **INVITED**

Graphene demonstrates exceptional properties such as high charge carrier mobility and high saturation velocity. Such attributes make graphene a promising candidate for radio frequency (rf) applications. However, one of the key limitations to the realization of graphene's full potential comes from its interaction with dielectric overlayers and metal contacts, which act to limit the excellent charge transport properties of graphene. We have directly demonstrated the importance of buffer elimination at the graphene/SiC(0001) interface where enhanced carrier mobilities of $>3000 \text{ cm}^2/\text{Vs}$ across large scale wafers is possible. Additionally, we have developed a robust method for forming high quality ohmic contacts to graphene, which improves the contact resistance by $>1000\times$ compared to untreated metal/graphene interfaces. We have also developed methods for ultra-thin gate oxides, and will discuss integration and the importance on improved interfaces between the graphene and dielectric. Each of these developments have provided a means to achieve graphene transistors with current saturation values $>1.5 \text{ A/mm}$, transconductance $> 400\text{mS}$, impressive *extrinsic* current gain response of epitaxial graphene transistors ($>30 \text{ GHz}$), and *intrinsic* current gain nearing 150 GHz . Additionally, we analyze the third order intermodulation product, gain compression and high frequency noise performance of graphene transistors for low noise amplifier applications and benchmark the graphene transistors with other RF device technologies. The graphene amplifier (un-matched) exhibits an output third order intercept (OIP3) of 19dBm and input 1dB gain compression ($P_{in,1dB}$) of 5.6dBm . Finally, the performance of a graphene mixer will be discussed and evidence is provided that matched graphene mixers can outperform current state-of-the-art technologies.

9:00am GR+EM+MS+NS+SP-FrM3 Direct Transfer of Graphene Devices on Arbitrary Substrates, **Z. Razavi Hesabi**, C.A. Joiner, T. Roy, E.M. Vogel, Georgia Institute of Technology

The wide-ranging high performance electronic properties of graphene and its ability to be roll-to-roll manufactured, provides an interesting platform for developing high performance, multifunctional electronics on arbitrary substrates such as paper or plastic. However, these substrates are not compatible with conventional high-temperature semiconductor processing. In this work, graphene devices are fabricated on as-synthesized graphene on copper foil using conventional semiconductor device processing techniques. The fully fabricated devices are then transferred onto the substrate of interest (glass, paper, or plastic) using a conventional PMMA-based wet transfer method. The effect of devices designs and processing conditions such as metal contact area and type (top contact versus mixed edge/top contact) on graphene device performance is investigated. The obtained results show that for top contacts, the Dirac point cannot be observed, while for mixed edge/top contacts, the Dirac point is observed. The obtained results suggest metal doping and edge contact can significantly shift the Dirac point. Overall, the results demonstrate a novel method for fabricating high performance graphene devices on arbitrary substrates.

Key words: Graphene, Field Effect Transistor (FET), Direct Transfer

9:20am GR+EM+MS+NS+SP-FrM4 1/f Noise in Epitaxial Graphene Field Effect Transistors using Al_2O_3 and HfO_2 High k -Dielectrics, **H.K. Chan**, Newcastle Univ., UK, **V.D. Wheeler**, U.S. Naval Research Laboratory (NRL), **V.K. Nagareddy**, Newcastle Univ., UK, **L.O. Nyakiti**, NRL, **A. Nath**, George Mason Univ., **R.L. Myers-Ward**, **Z. Robinson**, **N.Y. Garces**, NRL, **M.V. Rao**, George Mason Univ., **J.P. Goss**, **N.G. Wright**, Newcastle Univ., UK, **C.R. Eddy, Jr.**, NRL, **A.B. Horsfall**, Newcastle Univ., UK, **D.K. Gaskill**, NRL

It has been shown that graphene has substantially low 1/f noise, a characteristic potentially advantageous for electronic sensor applications. Most reports have been from studies of devices on flakes, which lack the desirable scale-up potential for practical applications. Here, we report the 1/f noise behavior for gated graphene devices formed on SiC substrates using low pressure sublimation (LPS) of Si in an Ar ambient. In general, we found that the 1/f characteristics of LPS graphene to be similar to or superior to all prior studies.

The LPS graphene was synthesized in an Aixtron VP508 reactor on $\sim 2.5 \text{ cm}^2$ nominally on-axis 6H(0001) semi-insulating substrates from the same boule. The process was designed to produce nominally 1 ML of graphene on the terraces of the samples; the samples should be identical as the synthesis process has been demonstrated to be uniform and run-to-run reproducible. Samples were processed using typical photolithographic methods before dielectric deposition; a Ti/Au stack was used for ohmic and gate contacts. High-k dielectric deposition was accomplished via a two-step process that includes functionalization of graphene by Fluorine followed by atomic layer deposition (ALD) of 20 nm thick Al_2O_3 and HfO_2 . Previously, we have shown that F-functionalization results in pinhole-free coverage of dielectrics and the films possess Dirac voltage shifts of 0.5V and 1.5V and dielectric constants of 9 and 18, for Al_2O_3 and HfO_2 , respectively. The 1/f noise data was acquired using a fast Fourier transform analyzer coupled with low noise amplifier and was averaged over 5 different samples on the same substrate for each oxide case; V_{GS} was controlled forward and reverse in the range -3 to 2V.

The 1/f noise magnitude, S_f/f^2 , was found to scale with channel dimension and was comparable or smaller in magnitude to reports by others on graphene flakes thus suggesting that the underlying SiC and interface layer does not add an appreciable number of noise generation sites. Comparing samples with a gate oxide to those processed identically but without oxide shows the noise magnitude was similar implying that the F-functionalization-based ALD process does not degrade the graphene channel by inducing interfacial traps. For the gated samples, the composition of the gate oxide had a minor effect on the channel noise magnitude relative to non-gated samples. For HfO_2 devices having an oxide surface coverage of $20 \times 4 \text{ m}^2$, $S_f/f^2 = 4 \times 10^{-11} \text{ Hz}^{-1}$ (at 20 Hz). For gated measurements, the 1/f noise magnitude were not flat but showed a slight (20%) dependence on V_{GS} . Both oxides showed noise hysteresis ($\sim 15\%$) although it was more pronounced for the HfO_2 devices.

9:40am GR+EM+MS+NS+SP-FrM5 MoS₂ MOSFETs: Dielectrics, Metal Contacts and Scaling, **P.D. Ye**, Purdue University **INVITED**

The discovery of graphene has unveiled another material family with layered structures, which includes boron nitride, topological insulators such as Bi_2Te_3 and Bi_2Se_3 , and transition metal dichalcogenides like MoS_2 , WS_2 , and NbSe_2 . Though graphene, a fascinating two-dimensional (2D) crystal, has shown a superior carrier mobility of up to $200,000 \text{ cm}^2/\text{V}\cdot\text{s}$, its zero bandgap property limits its application to logic devices as graphene transistors cannot have high on/off ratios. As opposed to the semi-metal graphene, transition metal dichalcogenides (such as MoS_2), as another type of layered structure material, have shown great potential in device applications due to their satisfied bandgaps, thermal stability, carrier mobility, and compatibility to silicon CMOS process. In order to realize high performance MoS_2 MOSFETs [1], three major issues must be solved: 1) how to deposit a high-quality dielectric on 2D crystal, 2) the fabrication of low-resistivity metal-semiconductor junction to be used as device contacts, and 3) the elimination of short channel effects. [2,3] In this talk, I will review the recent progress in this field about these three device aspects and discuss the fundamental physics, chemistry, and possible solutions on these challenges.

The work is in close collaborations with H. Liu, A.T. Neal, and Y.C. Du. The authors appreciate SRC GRC for the support.

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[2] Liu, H.; Neal, A.T.; Ye, P.D. Channel Length Scaling of MoS_2 MOSFETs, *ACS Nano* 2012, 6, 8563-8569.

[3] Liu, H.; Ye, P.D. MoS_2 Dual-Gate MOSFET with Atomic-Layer-Deposited Al_2O_3 as Top-Gate Dielectric, *IEEE Electron Device Lett.* 2012, 33, 546-548.

10:20am GR+EM+MS+NS+SP-FrM7 Broad Band Dielectric Functions of Graphene and MoS₂, **W. Li**, **G. Cheng**, National Institute of Standards and Technology (NIST), **Y. Liang**, Peking Univ., China, **K. Xu**, NIST, **A. Boosalis**, Univ. of Nebraska-Lincoln, **P.D. Ye**, Purdue Univ., **A.R. Hight Walker**, NIST, **X. Liang**, Peking Univ., China, **T. Hofmann**, Univ. of Nebraska-Lincoln, **C.A. Richter**, **D.J. Gundlach**, **N.V. Nguyen**, NIST

Graphene and MoS_2 are among the most promising candidates for next generation of electronic and photonic devices. Accurate optical properties provide key information necessary for electronic and photonic device design. Here, we report the results of a broad band optical measurement of the dielectric function by spectroscopic ellipsometry (SE) of graphene and MoS_2 grown by chemical vapor deposition (CVD). With the extended spectral range, we are able to observe new higher energy interband absorptions in MoS_2 and a red shift of graphene excitons.

Monolayer graphene grown on a copper foil was transferred onto a fused silica substrate by solvent method; two and three graphene layers were formed by the sequential transfer of each monolayer. MoS₂ was directly grown on sapphire. Raman spectroscopy was performed on each sample. Both the exciton peak (around 4.8 eV) and another absorption peak (around 6.3 eV) were observed from the absorption spectra of graphene. In the IR range, both refractive index (n) and k increase with longer wavelength which is consistent with the reported results.^(a) It is notable that n increases whereas k decreases as the number of graphene layers increases. This is most likely due to the relatively weak interaction between transferred graphene monolayers. More importantly, we observe a red shift of the exciton peak for two layer graphene (0.04 eV shift) and three layer graphene (0.07 eV shift) relative to that of monolayer graphene, which we attribute to the interlayer screening effects. The theory predicts^(b) the transmittance of monolayer graphene to depend solely on the universal fine structure constant $\alpha = e^2/hc$, which is related to the graphene's opacity. We find opacity to linearly increase for each of added layer. For example, at 550 nm the transmittance of one, two, and three layers of graphene are 96.9%, 93.6%, and 90.3%, respectively. Raman studies on MoS₂ confirm the presence of 3 layers, consistent with the three layer model derived from ellipsometry. The MoS₂ dielectric function exhibits the well-known A (1.86 eV) and B (2.02 eV) strong excitons which arise from the direct d-d transitions separated by a spin-orbit splitting. A series of higher energy interband transitions are clearly seen at 2.8, 3.1, 4.7 eV of which the 2.8 eV peak is the strongest absorption peak ever reported for MoS₂.

(a) F. J. Nelson, et al., Appl. Phys. Lett. 97, 253110 (2010)

(b) A. B. Kuzmenko, E. van Heumen, F. Carbone, and D. van der Marel, PRL **100**, 117401 (2008); R. R. Nair, P. Blake, A. N. Grigorenko, K. S. Novoselov, T. J. Booth, T. Stauber, N. M. R. Peres, A. K. Geim, *Science* **320**, 1308 (2008).

10:40am **GR+EM+MS+NS+SP-FrM8 Measurement of Charge Doping of Graphene in a Metal/Graphene/Dielectric Sandwich Structure by C-1s Core Level X-ray Photoelectron Spectroscopy.** A. Dahal, M. Batzill, R. Addou, H. Coy-Diaz, J. Lallo, University of South Florida

The contact resistance between graphene and metals critically affects device operations. In most realistic graphene device structures, graphene is supported on an insulating substrate and metals are deposited on top of graphene to make electrical contacts. Thus we should evaluate the contact resistance of a metal/graphene/dielectric sandwich structure rather than just a metal/graphene interface. A critical component for evaluating the contact resistance is the Fermi-level shift in graphene underneath the metal contact. We show that this Fermi-level shift relative to the graphene's Dirac point, can be measured from C-1s core level x-ray photoelectron spectroscopy (XPS). In XPS of solids the binding energy is referenced to the Fermi-level, consequently measurement of C-1s core level of graphene allows us, in the absence of chemical shifts, to determine the Fermi-level of graphene at metal/graphene interfaces as well as at metal/graphene/dielectric interfaces. We show that the Fermi-level shift for metal/graphene interfaces of the weakly interacting metals such as Pt, Ir, Al, and Cu agrees well with previously reported DFT calculations(ref.1). However, the Fermi-level shift of graphene is strongly altered if graphene is sandwiched between a metal and a dielectric oxide. This behavior can be explained by a modified Schottky contact model. In metal/graphene/oxide sandwich structure, metal is replaced by a graphene/metal heterostructure and thus charges in the Schottky contact will be located on the graphene. A simple capacitor model for graphene/oxide interfaces predicts the difference in charge doping for graphene on a metal compared to graphene sandwiched between a metal and dielectric as $\Delta E_F \approx 0.2 \times (\Phi_{\text{metal}} - \Phi_{\text{dielectric}})$, in good agreement with our measurements.

Key words: Interface, Doping, Fermi-level, Spectroscopy, Schottky contact

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Authors Index

Bold page numbers indicate the presenter

— A —

Abdallah, J.: MS+AS+EL+EM+PS+TF-TuA4, 4
Addou, R.: GR+EM+MS+NS+SP-FrM8, 12
Arnold, J.C.: MS+AS+EL+EM+PS+TF-TuA9, 4
Astier: MS+AS+BA+BI+PS+TF-TuM3, 3

— B —

Bae, D.: MS+AS+EL+EM+PS+TF-TuA9, 4
Bai, J.: MS+AS+BA+BI+PS+TF-TuM3, 3
Bai, Q.: MS+AS+BA+BI+PS+TF-TuM1, 3
Bailey, S.: MS+AS+BA+BI+PS+TF-TuM11, 3
Banik, A.: MS+AS+EL+EM+PS+TF-TuA9, 4
Batzill, M.: GR+EM+MS+NS+SP-FrM8, 12
Bentley, S.: MS+AS+EL+EM+PS+TF-TuA9, 4
Bez, R.: MS+AS+EM+NS+PS+TF-MoA8, 2
Boosalis, A.: GR+EM+MS+NS+SP-FrM7, 11
Bower, S.: MS+AS+BA+BI+PS+TF-TuM11, 3
Brennen, R.: MS+AS+BA+BI+PS+TF-TuM1, 3
Brink, M.: MS+AS+BA+BI+PS+TF-TuM3, 3
Broadbridge, C.C.: MG+EN+MS-WeA1, 9
Bruce, R.L.: MS+AS+BA+BI+PS+TF-TuM3, 3
Butler, J.: MS+AS+BA+BI+PS+TF-TuM11, 3

— C —

Carr, L.: MS+AS+BA+BI+PS+TF-TuM1, 3
Ceder, G.: MG+EM+MI+MS-WeM9, 7
Chan, B.T.: MS+AS+EM+NS+PS+TF-MoA6, 2
Chan, H.K.: GR+EM+MS+NS+SP-FrM4, 11
Cheng, G.: GR+EM+MS+NS+SP-FrM7, 11
Chu, N.: MS-TuP2, 6
Colburn, M.E.: MS+AS+EL+EM+PS+TF-TuA4, 4
Cole, C.: MS+AS+EL+EM+PS+TF-TuA9, 4
Colombo, L.: MS+AS+EM+NS+PS+TF-MoA1, 2
Cotte, J.: MS+AS+BA+BI+PS+TF-TuM3, 3
Coy-Diaz, H.: GR+EM+MS+NS+SP-FrM8, 12
Crabtree, G.: MS+AS+EM+EN+NS+TF-MoM1, 1

— D —

Dahal, A.: GR+EM+MS+NS+SP-FrM8, 12
de Pablo, J.J.: MG+EM+MI+MS-WeM3, 7

— E —

Eddy, Jr., C.R.: GR+EM+MS+NS+SP-FrM4, 11
Ediger, M.D.: MG+EM+MI+MS-WeM3, 7
Eom, C.: MG+EM+MI+MS-WeM11, 7
Estrada-Raygoza, I.C.: MS+AS+EL+EM+PS+TF-TuA4, 4

— F —

Farah, S.: MS+AS+BA+BI+PS+TF-TuM11, 3
Farrar, P.: MS+AS+EM+NS+PS+TF-MoA10, 2
Flatt, J.: MS+AS+BA+BI+PS+TF-TuM11, 3

— G —

Garces, N.Y.: GR+EM+MS+NS+SP-FrM4, 11
Gaskill, D.K.: GR+EM+MS+NS+SP-FrM4, 11
Gibson, D.: MS+AS+BA+BI+PS+TF-TuM11, 3
Gignac: MS+AS+BA+BI+PS+TF-TuM3, 3
Ginley, D.: MG+EM+MI+MS-WeM6, 7
Goldblatt: MS+AS+BA+BI+PS+TF-TuM3, 3
Goss, J.P.: GR+EM+MS+NS+SP-FrM4, 11
Gouma, P.: MS+AS+EL+EM+PS+TF-TuA10, 4
Gronheid, R.: MS+AS+EM+NS+PS+TF-MoA6, 2
Guillorn, M.: MS+AS+BA+BI+PS+TF-TuM3, 3
Gundlach, D.J.: GR+EM+MS+NS+SP-FrM7, 11

— H —

Haensch, W.: MS+AS+EM+NS+PS+TF-MoA3, 2
Hannon, J.: MS+AS+BA+BI+PS+TF-TuM11, 3
Haran, B.: MS+AS+EL+EM+PS+TF-TuA9, 4
Harris, S.: MS+AS+EM+EN+NS+TF-MoM10, 1

Henderson, C.: MS+AS+EL+EM+PS+TF-TuA3, 4
Hight Walker, A.R.: GR+EM+MS+NS+SP-FrM7, 11
Hofmann, T.: GR+EM+MS+NS+SP-FrM7, 11
Horsfall, A.B.: GR+EM+MS+NS+SP-FrM4, 11
Hsieh, F.C.: MS-TuP2, 6
Huang, C.Y.: MS-TuP2, 6

— I —

Ito, K.: MS+AS+EL+EM+PS+TF-TuA9, 4

— J —

Jahnes, C.: MS+AS+BA+BI+PS+TF-TuM3, 3
Jang, L.: MS+AS+EL+EM+PS+TF-TuA9, 4
Johnson, D.: MS+AS+EM+EN+NS+TF-MoM8, 1
Joiner, C.A.: GR+EM+MS+NS+SP-FrM3, 11
Joseph, E.A.: MS+AS+BA+BI+PS+TF-TuM3, 3
Jung, R.: MS+AS+EL+EM+PS+TF-TuA9, 4

— K —

Kanakasabapathy, S.: MS+AS+EL+EM+PS+TF-TuA9, 4
Kang, H.: MS+AS+EL+EM+PS+TF-TuA9, 4
Kao, J.S.: MS-TuP2, 6
Killeen, K.: MS+AS+BA+BI+PS+TF-TuM1, 3
Kinlen, P.: MG+EN+MS-WeA9, 9
Ko, A.: MS+AS+EL+EM+PS+TF-TuA4, 4;
MS+AS+EL+EM+PS+TF-TuA9, 4
Krishnan, M.: MS+AS+BA+BI+PS+TF-TuM3, 3
Kumar, K.: MS+AS+EL+EM+PS+TF-TuA9, 4

— L —

Laderman, S.: MS+AS+BA+BI+PS+TF-TuM5, 3
Lallo, J.: GR+EM+MS+NS+SP-FrM8, 12
Lampenscherf, S.: MG+EN+MS-WeA3, 9
Lany, S.: MG+EM+MI+MS-WeM5, 7;
MG+EM+MI+MS-WeM6, 7
Lawson, R.: MS+AS+EL+EM+PS+TF-TuA3, 4
Li, W.: GR+EM+MS+NS+SP-FrM7, 11
Liang, X.: GR+EM+MS+NS+SP-FrM7, 11
Liang, Y.: GR+EM+MS+NS+SP-FrM7, 11
Lie, F.L.: MS+AS+EL+EM+PS+TF-TuA9, 4
Lin, P.H.: MS-TuP2, 6
Lin, Q.: MS+AS+BA+BI+PS+TF-TuM3, 3
Liu, C.: MS+AS+EL+EM+PS+TF-TuA4, 4
Lofaro, M.: MS+AS+BA+BI+PS+TF-TuM3, 3
Lozano, K.: MS+AS+EL+EM+PS+TF-TuA11, 5
Ludovice, P.: MS+AS+EL+EM+PS+TF-TuA3, 4

— M —

Marder, M.: MG+EN+MS-WeA11, 10
Martinez, L.: MS+AS+BA+BI+PS+TF-TuM1, 3
Metz, A.: MS+AS+EL+EM+PS+TF-TuA9, 4
Mignot, S.: MS+AS+EL+EM+PS+TF-TuA4, 4
Mihut, D.M.: MS+AS+EL+EM+PS+TF-TuA11, 5
Mohanti, N.: MS+AS+EL+EM+PS+TF-TuA4, 4
Molnar, M.: MS+AS+EM+EN+NS+TF-MoM3, 1
Moon, Y.: MS+AS+EL+EM+PS+TF-TuA9, 4
Morris, B.G.: MS+AS+EL+EM+PS+TF-TuA4, 4
Myers-Ward, R.L.: GR+EM+MS+NS+SP-FrM4, 11

— N —

Nagareddy, V.K.: GR+EM+MS+NS+SP-FrM4, 11
Nam: MS+AS+BA+BI+PS+TF-TuM3, 3
Nath, A.: GR+EM+MS+NS+SP-FrM4, 11
Nealey, P.F.: MS+AS+EM+NS+PS+TF-MoA6, 2
Nguyen, N.V.: GR+EM+MS+NS+SP-FrM7, 11
Nyakiti, L.O.: GR+EM+MS+NS+SP-FrM4, 11

— P —

Papa Rao, S.: MS+AS+BA+BI+PS+TF-TuM3, 3

Peng, H.: MG+EM+MI+MS-WeM5, 7
Perkins, J.: MG+EM+MI+MS-WeM6, 7
Peters, A.: MS+AS+EL+EM+PS+TF-TuA3, 4
Pollentier, I.: MS+AS+EM+NS+PS+TF-MoA6, 2
Post, S.: MS+AS+BA+BI+PS+TF-TuM1, 3
Prieto, A.: MS+AS+EM+EN+NS+TF-MoM8, 1

— R —

Raley, A.: MS+AS+EL+EM+PS+TF-TuA4, 4
Ranjan, A.: MS+AS+EL+EM+PS+TF-TuA9, 4
Rao, M.V.: GR+EM+MS+NS+SP-FrM4, 11
Rastogi, V.: MS+AS+EL+EM+PS+TF-TuA4, 4
Razavi Hesabi, Z.: GR+EM+MS+NS+SP-FrM3, 11
Reuter: MS+AS+BA+BI+PS+TF-TuM3, 3
Richter, C.A.: GR+EM+MS+NS+SP-FrM7, 11
Rincon Delgadillo, P.A.:
MS+AS+EM+NS+PS+TF-MoA6, 2
Ritchey, D.: MS+AS+BA+BI+PS+TF-TuM1, 3
Robinson, J.A.: GR+EM+MS+NS+SP-FrM1, 11
Robinson, Z.: GR+EM+MS+NS+SP-FrM4, 11
Rosnagel, S.M.: MS+AS+BA+BI+PS+TF-TuM3, 3
Rossner, W.: MG+EN+MS-WeA3, 9
Roy, T.: GR+EM+MS+NS+SP-FrM3, 11

— S —

Sapper, E.: MG+EN+MS-WeA9, 9
Seaward, K.: MS+AS+BA+BI+PS+TF-TuM1, 3
Seo, S.: MS+AS+EL+EM+PS+TF-TuA9, 4
Smith: MS+AS+BA+BI+PS+TF-TuM3, 3
Sood, S.: MS+AS+EL+EM+PS+TF-TuA10, 4
Staples, G.: MS+AS+BA+BI+PS+TF-TuM1, 3
Stevanovic, V.: MG+EM+MI+MS-WeM5, 7;
MG+EM+MI+MS-WeM6, 7
Stolovitsky: MS+AS+BA+BI+PS+TF-TuM3, 3
Sundaram, G.M.: MS+AS+EM+EN+NS+TF-MoM5, 1

— T —

Turner, S.: MS+AS+BA+BI+PS+TF-TuM9, 3

— V —

Van Look, L.: MS+AS+EM+NS+PS+TF-MoA6, 2
Vogel, E.M.: GR+EM+MS+NS+SP-FrM3, 11
Voronin, S.: MS+AS+EL+EM+PS+TF-TuA9, 4

— W —

Wang: MS+AS+BA+BI+PS+TF-TuM3, 3
Wheeler, V.D.: GR+EM+MS+NS+SP-FrM4, 11
Windl, W.E.: MG+EN+MS-WeA7, 9
Wong, H.-S.P.: MS+AS+EL+EM+PS+TF-TuA1, 4
Wright, N.G.: GR+EM+MS+NS+SP-FrM4, 11

— X —

Xu, K.: GR+EM+MS+NS+SP-FrM7, 11

— Y —

Ye, P.D.: GR+EM+MS+NS+SP-FrM5, 11;
GR+EM+MS+NS+SP-FrM7, 11
Yi, H.: MS+AS+EL+EM+PS+TF-TuA1, 4
Yin, H.: MS+AS+BA+BI+PS+TF-TuM1, 3
Yin, Y.: MS+AS+EL+EM+PS+TF-TuA4, 4;
MS+AS+EL+EM+PS+TF-TuA9, 4
Younkin, T.R.: MS+AS+EM+NS+PS+TF-MoA6, 2
Yu, L.: MG+EM+MI+MS-WeM3, 7

— Z —

Zakutayev, A.: MG+EM+MI+MS-WeM6, 7
Zhao, W.: MS+AS+EL+EM+PS+TF-TuA11, 5