

Thursday Evening Poster Sessions

2D Materials Focus Topic

Room: Central Hall - Session 2D-ThP

2D Materials Poster Session

2D-ThP1 In-situ Analysis of Electronic Structure of monolayer MoS₂ using Photoemission Spectroscopy and Kelvin probe. *JaeGwan Chung, U.J. Kim, D. Yun, Y.S. Kim, J. Shin*, Samsung Electronics, Republic of Korea

Although two-dimensional monolayer transition metal dichalcogenides reveal numerous unique features that are inaccessible in bulk materials, their intrinsic properties are often obscured by environmental effects. Among them, work function, which is the energy required to extract an electron from a material to vacuum, is one critical parameter in electronic/optoelectronic devices.

In this study, we systematically measure the electronic structure of monolayered MoS₂ – work function, energy band gap, conduction band and valence band structure by in-situ photoemission spectroscopy (PES), inverse photoemission spectroscopy (IPES), reflective electron energy loss spectroscopy (REELS) and Kelvin Probe (KP) under various ambient condition (air, ultra-high vacuum, oxygen and nitrogen gases). The energy band gap by REELS of monolayer MoS₂ on SiO₂ is 1.7 eV. It shows a increase as compared with the optical band gap of 1.2 eV of Bulk MoS₂ [1]. And also, the valence band offset and conduction band offset of mono layer MoS₂ are shifted higher binding energy side of 0.5 eV. A work function measured by in-situ KP of 4.04 eV in vacuum was converted to 4.47 eV with O₂ exposure, which is comparable with a large variation in graphene. The homojunction diode by partially passivating a transistor reveals an ideal junction with an ideality factor of almost one and perfect electrical reversibility. The estimated depletion width obtained from photocurrent mapping was ~200 nm, which is much narrower than bulk semiconductors. References

[1] Y. Zhang, Nature nanotech. **9** 111 (2014).

2D-ThP2 Reliable Passivation of Black Phosphorus by Thin Hybrid Coating. *S. Gamage, Alireza Fali, N. Aghamiri*, Georgia State University, *L. Yang, P.D. Ye*, Purdue University, *Y. Abate*, Georgia State University
Topic: 2D materials

Black phosphorus (BP) possesses several extraordinary properties such as layered structure but with a unique puckered single-layer geometry, thickness dependent direct bandgap, high carrier mobility and anisotropic in-plane properties that not shared by other exfoliable materials that are highly desirable from the point of view of fundamental science and modern optoelectronics applications. The excitement about this material has always been accompanied by unreserved skepticism due to its extraordinary degradation under ambient conditions. Here we show ambient degradation of exfoliated BP can be effectively suppressed using thin layer of hybrid MOCVD coating of BN followed by ALD coating of Al₂O₃. We have extensively studied the time dependent surface, optical and electrical properties of BP encapsulated by BN and/or Al₂O₃ using nanoscale infrared imaging and I-V characterizations. Our results show hybrid thin layer (~5 nm) BN/Al₂O₃ coated BP exfoliated on SiO₂ substrate is protected from degradation in ambient for over 45 days much longer than those coated on BN or Al₂O₃ layers only as well as those exfoliated on Si substrate. Our theoretical modeling of the experimental degradation growth pattern shows that the influence of neighboring elements on the degradation of a given element is minimal for BP flakes with hybrid coating. Electrical characterization further confirms the effectiveness of BN/Al₂O₃ as encapsulation layer and gate dielectrics with minor changes after several weeks.

2D-ThP3 Temperature-dependent Photo-current Behaviors of CVD-grown MoS₂ layers. *Soyeong Kwon, E. Kim, Y. Cho*, Ewha Womans University, Republic of Korea, *Y. Kim, B. Cho, D.-H. Kim*, Korea Institute of Materials Science, *D.-W. Kim*, Ewha Womans University, Republic of Korea
MoS₂, a representative 2D atomically thin semiconductor, has unique optical, electrical, and mechanical properties. There have been intensive research efforts to fabricate MoS₂-based optoelectronic devices due to its sizable band gap (1.2 ~ 1.8 eV). In this work, we investigated transport behaviors of MoS₂ layers, grown by chemical vapor deposition (CVD), in dark and under illumination of visible light [1,2]. CVD techniques can produce high-quality, large-area MoS₂ thin films with a high throughput. Surface potential maps near the electrode/MoS₂ contacts were obtained using Kelvin probe force microscopy, which clearly showed how the potential gradient near the contacts could affect the collection of the photo-generated carriers. The dark- and photo-current behaviors of the devices in dark and light were measured

while varying the sample temperature (100 ~ 300 K). The temperature dependent current-voltage characteristics helped us to understand the carrier transport mechanism and its roles in the photo-detection of the CVD-grown MoS₂ thin films.

1. Y. Cho et al., *ACS Appl. Mater. Interfaces* **8**, 21612 (2016).

2. Y. Cho et al., *ACS Appl. Mater. Interfaces* **9**, 6314 (2017).

2D-ThP4 Controlling Charge Density Wave Transition in Monolayer TiSe₂. *Sadhu Kolekar, M. Batzill*, University of South Florida

Layered transition metal dichalcogenides (TMDCs) have been studied for their charge density wave (CDW) and superconductivity transitions. TiSe₂ is interesting because traditional explanations for CDW formation based on electron phonon coupling described by Fermi surface nesting does not apply. Instead an unconventional excitonic mechanism has been invoked. The well-established dependence of the exciton binding energy on the number of layers in TMDCs implies that the CDW transition in TiSe₂ should also be layer dependent. Furthermore, the dielectric properties of the substrate for monolayer TiSe₂ should exert further control over the excitonic properties and thus the CDW transitions in TiSe₂. Here we investigate mono- to few-layer TiSe₂ films grown by molecular beam epitaxy on HOPG or MoS₂ substrate by variable temperature scanning tunneling spectroscopy. We show that the band gap opening and CDW transition temperature in monolayer is strongly increased compared to bulk TiSe₂ and correlates with the expected exciton binding energy dependence. Interestingly, we also observe phase coherence peaks in monolayer TiSe₂. The phase coherence occurs, however, at a much lower temperature than the CDW transition, suggesting that formation of an excitonic condensate is possible but is not essential for CDW formation.

2D-ThP5 Growth and Characterization of MoTe₂ on GaTe by Molecular Beam Epitaxy. *Paula Mariel Coelho, M. Batzill*, University of South Florida

MoTe₂ exist in semiconducting (2H) and metallic (1T') polymorphs. The potential for switching between these phases makes it a promising 2D material for phase change applications. In this study we are investigating van der Waals epitaxy of single layer MoTe₂ on different substrates and growth conditions. Specifically, we aim at selectively growing 2H or 1T' phases by molecular beam epitaxy. Using van der Waals substrates with symmetries similar to the 2H or 1T' phases of MoTe₂ we are aiming at obtaining epitaxial single crystalline monolayer materials. Specifically, we propose GaTe to be a suitable substrate for the growth of 1T'-MoTe₂. We characterize the substrates and MoTe₂-films *in-situ* by scanning tunneling microscopy (STM), x-ray photoelectron spectroscopy (XPS) and angle resolved photoemission spectroscopy (ARPES). Furthermore the thermal stability and phase change behavior of these monolayers are investigated.

2D-ThP7 Single Layer VSe₂: A Ferromagnetic 2D Material. *Manuel Bonilla, S. Kolekar, H. Coy Diaz, Y. Ma, M. Batzill*, University of South Florida

VSe₂ has been proposed to be ferromagnetic in single- to few- layer form. However, the high reactivity of VSe₂ makes mechanical exfoliation to single layers and subsequent magnetic characterization challenging. Here we grow VSe₂ by molecular beam epitaxy in ultra-high vacuum. We characterize the film-growth and materials properties *in-situ* by scanning tunneling microscopy/spectroscopy and photoemission spectroscopy. High quality single- to few- layer materials are obtained, with the well-known charge density wave transition for bulk VSe₂ persisting to monolayer material. For magnetic characterizations we protect the single- to few- layer materials from oxidation by a few nanometer thick selenium capping layer. We observe a strong ferromagnetism for the single layer, which decreases with number of layers. This study shows that VSe₂ single layer is indeed a promising 2D ferromagnetic material, whose magnetic properties can be tuned by the layer thickness.

2D-ThP8 Surface Functionalization of Few-layer MoS₂ for Atomic Layer Deposition using Gold Chloride Salts. *Jaron Kropp, T. Gougousi*, University of Maryland, Baltimore County

Transition metal dichalcogenides such as MoS₂ have attracted much interest in the field of nanoelectronics in recent years. MoS₂ is a layered material with a hexagonal structure similar to graphene. Unlike graphene, however, MoS₂ is a semiconducting material with an indirect band gap of ~1.2 eV in bulk form and a direct band gap of ~1.8 eV in monolayer form. As such, MoS₂ has attracted interest as a possible channel material in field-effect transistors. An important feature of the modern field-effect transistor is the gate dielectric. In the past decade, the electronics industry has transitioned from using native silicon oxide as the gate dielectric to using high-k metal oxides deposited via atomic layer deposition. Field-effect devices fabricated from MoS₂ will thus

require the growth of metal oxides on the MoS₂ surface. Unfortunately, the sulfur-terminated MoS₂ surface is hydrophobic and not conducive to metal oxide film growth using atomic layer deposition. As such, the surface must be functionalized prior to deposition. Here, we report a novel wet chemistry method for functionalization of MoS₂ surfaces using gold chloride salts.

Mechanically exfoliated MoS₂ surfaces are treated by immersion in a solution of HAuCl₄ or AuCl₃ for 5-60 seconds and are subsequently subjected to atomic layer deposition of Al₂O₃ using trimethylaluminum and water as precursors. We measure the effectiveness of the surface treatment by investigating the post-deposition surface topography using atomic force microscopy. Our hypothesis is that immersion of the MoS₂ surfaces in the gold chloride solution will leave behind adsorbed gold chloride molecules which render the surface hydrophilic and amenable to the growth of metal oxide films. While untreated surfaces show island growth, gold chloride-treated surfaces show more coalesced films. Treatment for at least 30 seconds results in a reduction of the film RMS roughness by a factor of 4 compared to untreated surfaces after deposition of 3 nm (nominal thickness) Al₂O₃ at 200°C. Film surface coverage improves from 50-60% on untreated surfaces to 80-99% on surfaces treated for 10 seconds and finally to complete film coverage on surfaces treated for 30 and 60 seconds. Surface roughness and coverage is investigated as a function of film thickness and deposition temperature, and provides information on initial growth mechanisms and process conditions for the growth of conformal, high-quality films.

2D-ThP10 Alternative Pathway to Silicene Synthesis via Surface Relaxation of Hexagonal-MoSi₂ Crystallites, Cameron Volders, E. Monazami, G. Ramalingam, P. Reinke, University of Virginia

The 2D material community has been dominated by Graphene, however, more recently, different single layer materials have garnered more attention including transition metal dichalcogenides (TMDs), silicene, and germanene. Silicene is particularly intriguing due to its potential for integration into silicon based devices. The most frequently used method for synthesizing silicene has been the deposition of monolayer (ML) amounts of Si onto Ag (111). The resulting layer(s) exhibit a honeycomb symmetry, which have been identified as silicene. An alternative interpretation of the Si-Ag system suggests the formation of 2D Ag-Si surface alloy rather than the formation of a well-defined silicene layer.

Our work will present an approach, which offers an alternative pathway for growing silicene layers, based on the observation of a Silicene-like reconstruction (SLR) on the surface of hexagonal-MoSi₂ crystallites. Scanning Tunneling Microscopy and Spectroscopy were the primary techniques used for this study. H-MoSi₂ crystallites are grown by depositing Mo onto a Si (001) surface followed by annealing. These crystallites are terminated by the (0001) plane which is comprised of Si hexagons with a Mo atom residing in the center. Upon annealing, the Si atoms decouple from the underlying h-MoSi₂ crystallites and a honeycomb pattern with the lateral dimensions of a low-buckled silicene structure is observed.

We first discuss the optimal parameter space where the SLR is consistently reproduced. This regime includes depositing 2-5 MLs of Mo onto a Si (001) substrate and annealing around 650 - 800°C. In this regime the SLR structure is readily observed and the geometrical parameters are nearly identical to that of a ($\sqrt{3}\times\sqrt{3}$) silicene superstructure. Additional features of the SLR such as a well-defined 'rim' structure and defect motif will also be discussed.

The area of the SLR structure is controlled by the surface area of the h-MoSi₂ crystallites, therefore, the second portion of this work will discuss how to control the size and distribution of these crystallites, thus the area of the SLR layer. This becomes critical for future device integration and assessing the detailed bonding structure with AR-UPS.

We would like to thank the Office of Naval Research for supporting this work.

(1) Volders, C.; Monazami, E.; Ramalingam, G.; Reinke, P. Alternative Route to Silicene Synthesis via Surface Reconstruction on h-MoSi₂ Crystallites *Nano. Lett.* **2017**, 17, 299-307.

2D-ThP11 CVD Grown 2D Metal Carbides using Folded Cu/Metal Foils, Kwonjae Yoo, I.S. Kang, G. Kim, M.S. Hyun, Y.C. Park, National Nanofab Center (KAIST), Republic of Korea, S. Lee, C. Hwang, Korea Research Institute of Standards and Science, Republic of Korea

Two dimensional (2D) metal carbides (MC) are recently entered in a playground of 2D materials world. Unlike conventional 2D materials, such as graphene and transition metal chalcogenides, they have shown the unique properties of 2D metallic- and superconducting- state. Moreover, their high thermal and chemical stability due to covalent-ionic bonding between metal and carbide atoms can offer a great advantage for harsh environmental sensor applications.

2D MC are obtained by selective extraction method from ternary carbides or by recently chemical vapor deposition (CVD). While monolayer metal

carbides known as MXenes which produced by selective extraction method have shown defects and surface terminations which affect their physical properties, CVD grown monolayer metal carbides such as Mo₂C, W₂C are known to have very low defects [1, 2]. This modified CVD method uses Cu foil on molybdenum foil with melted Cu and moly alloy surface near the temperature of the Cu melting point.

Here we present the CVD using Cu foil inside folded Mo foil for growing metal carbides. The folded Mo foil inside CVD quartz tube not only prevents from evaporation of melted Cu, but also provides uniform gas flow. These growth conditions seem to be positive effect on the growth of large area and uniform monolayer metal carbides such as Mo₂C and W₂C. We investigated CVD grown monolayer Mo₂C using electron back scattering diffraction (EDSD), tunneling electron microscopy (TEM), and low temperature electron transport. Growth results depending on Cu crystallographic orientation will be discussed.

References

1. Large-area high quality 2D ultrathin Mo₂C superconducting crystals, Chuan Xu, et al. *Nature materials*, Vol. 14, (2015)1135-1142
2. Controlled growth of ultrathin Mo₂C superconducting crystals on liquid Cu surface, Dechao Geng, et al., *2D Mater.* 4 (2017)011012.

2D-ThP12 Scanning Tunneling Microscopy and Spectroscopy of Wet Chemically Synthesized Porous Graphene Nanoribbons, Kaitlyn Parsons, A. Radocea, University of Illinois at Urbana-Champaign, M. Pour, University of Nebraska - Lincoln, T. Sun, N. Aluru, University of Illinois at Urbana-Champaign, A. Sinitskii, University of Nebraska - Lincoln, J.W. Lyding, University of Illinois at Urbana-Champaign

The bottom-up wet chemical synthesis of graphene nanoribbons (GNRs) opens interesting opportunities for tailoring the GNR structure with atomic precision [1]. Atomically precise porous GNRs are a new chemically synthesized variation for which the fabrication procedure yielding multiple pores in a single ribbon and the electronic details of the ribbon have not been reported. In this work, porous GNRs are dry contact transferred in ultrahigh vacuum to clean silicon and III-V semiconducting substrates and examined using UHV scanning tunneling microscopy (STM) and spectroscopy (STS). STM imaging confirms the expected porous structure and indicates a unique electronic feature at the graphene nanopores, and STS measurements indicate a 2.0 eV bandgap. These results are compared to first-principles DFT simulations in which an increased local density of states at the pores is predicted. A GW correction predicts a 3.24 eV bandgap. Illumination of pore effects in GNRs contributes to an increased understanding of the tunability of GNR electronic structure. Porous GNRs have potential applications in molecular filtration, detection and DNA sequencing.

References

- [1] Vo, T. H., Shekhirev, M., Kunkel, D. A., Morton, M. D., Berglund, E., Kong, L., Wilson, P. M., Dowben, P. A., Enders, A., and Sinitskii, A., *Nat. Commun.* 2014, 5, 3189.

2D-ThP13 Surfactant-Exfoliated 2D Molybdenum Disulphide (2D-MoS₂): The Role of Surfactant upon the Hydrogen Evolution Reaction, Simon Hutton, Kratos Analytical Limited, UK, S.J. Rowley-Neale, C.E. Banks, Manchester Metropolitan University, UK, C.J. Blomfield, S.J. Coultas, A.J. Roberts, J.D.P. Counsell, Kratos Analytical Limited, UK

Hydrogen, produced via the electrolysis of water, is a promising alternative to fossil fuels. Hydrogen may be transported in bulk from areas of energy production to areas of energy consumption and used to generate electricity directly in fuel cells. One of the major problems limiting the widespread take-up of hydrogen based technology is the high cost of platinum which is used as a catalytic electrode material in both water electrolysis and fuel cells.[1]

Recent research has focused on finding a more cost effective electrode materials to catalyse the Hydrogen Evolution Reaction (HER). Studies have shown that 2D Molybdenum disulphide (2D-MoS₂) can be used as an effective electrocatalyst towards the HER.[2] Surfactant (e.g. sodium cholate, SC) mediated aqueous liquid phase exfoliation is a common method of fabricating 2D-MoS₂ nanosheets. This method produces defect free flakes with nanometer lateral size (2D-MoS₂-SC).

This study investigates the effect of using sodium cholate to produce the 2D nanosheets (2D-MoS₂-SC) on the electrocatalytic behaviour towards the HER when compared to 2D-MoS₂ produced without a surfactant. The 2D-MoS₂-SC nanosheet surface was characterised using X-ray photoelectron spectroscopy. Electrocatalytic performance was evaluated by measuring the HER onset potentials, current densities and Tafel values.

2D-ThP14 Low Damage Layer-controlled Thinning of Black Phosphorus by a Low Energy Ar⁺ Ion Beam, Jinwoo Park, D.S. Kim, W.O. Lee, M.K. Mun, K.S. Kim, G.Y. Yeom, Sungkyunkwan University, Republic of Korea

Black phosphorus (BP) is one of the most interested two-dimensional (2D) layered materials due to their unique properties of energy band gap change from 0.3 eV (bulk) to 2.0 eV (monolayer) depending on the number of BP layers for the application of nanoelectronic devices. Currently, for the fabrication of 2D BP materials, a thinning technique from bulk material to 2D material needs to be used while controlling the removed layer thickness. In this study, low-damage layer thinning of BP was performed by using an Ar⁺ ion beam method and its BP thinning characteristics were investigated. By using the Ar⁺ ion energy of ~ 45 eV, the BP could be thinned with the thinning rate of ~ 5 Å/min down to bilayer without increasing the surface roughness and changing the chemical binding states. Back-gate BP field-effect transistors (FETs) fabricated with a BP thinned to bilayer ~ 10 layers by the Ar⁺ ion beam exhibited the electrical characteristics similar to those of pristine BP FETs such as a high-drain current and 7000 on/off ratio suggesting no electrical damage on the BP layers thinned by the low-energy Ar⁺ ion beam. Therefore, it is believed that the low energy Ar⁺ ion beam technique used in this study can precisely control thickness 2D materials like BP without any damages and can be a promising thinning method for fabricating 2D-based devices.

2D-ThP15 Controlled Growth of Multilayered Hexagonal Boron Nitride on Ni-Cu Alloys, Karthik Sridhara, Texas A&M University, *B.N. Feigelson, J.K. Hite,* US Naval Research Laboratory, *L.O. Nyakiti,* Texas A&M University Galveston

Hexagonal boron nitride (h-BN) has been frequently studied as a potential substrate and a tunnel dielectric for two-dimensional materials such as graphene and transition metal dichalcogenides. Large area (>1 cm²) single and multilayered h-BN films have been successfully grown using chemical vapor deposition (CVD) on various single crystal and polycrystalline transition metal substrates such as Cu, Ni, Pt, and Ag. Of these substrates, polycrystalline Cu followed by polycrystalline Ni are by far the most commonly used substrates for CVD growth. Despite the popularity of polycrystalline Cu and Ni for the growth of h-BN, controlled uniform growth of multilayered (>3 layers) and few-layered (<3 layers) h-BN still remains a challenge.

We propose a method to grow few and multilayered h-BN on nickel-copper (NiCu) alloys, and control the thickness of h-BN by varying the concentration of Cu in NiCu alloy samples. These NiCu alloys are prepared by electroplating Cu onto high purity (99.8%) Ni foils (25 μm) and thermally annealing them at 1030°C for > 3 hours in H₂ environment. The Cu concentration in the alloy can be controlled by the electroplating current density and time to give desired weight percent of Cu deposited on Ni foils. NiCu alloys with four different Cu weight percentages (10%, 20%, 30%, 40%) are prepared using electroplating and thermal annealing procedure. The alloyed foils are subsequently cut into smaller pieces (~1 cm²) and are further annealed before h-BN growth. h-BN films are grown on these alloyed samples at 1030°C using borazine as the precursor, with H₂ and N₂ as the carrier gases, and high purity Cu (99.98%) and Ni (99.8%) are used as control samples. We use energy dispersive spectroscopy (EDS) and X-ray photoelectron spectroscopy (XPS) to quantify the Ni and Cu concentration in the alloy. Scanning electron microscopy (SEM) is used to assess the surface morphology of the alloys, and ascertain the crystal size of h-BN films. We use Fourier transform grazing-incidence infrared reflection absorption spectroscopy (FT-IRRAS) to assess the h-BN film growth. Our preliminary results show that there is an immediate increase in the amount (thickness) of h-BN with the introduction of Cu in the NiCu alloy. We observe a subsequent decrease of h-BN thereafter with increasing Cu concentration in the NiCu alloy samples. We consistently observe that the thickest h-BN films, as calculated by FT-IRRAS peak area, grow on Ni₉₀Cu₁₀ while the thinnest grow on Ni₆₀Cu₄₀. We also observe that the alloy grain size decreases with increasing Cu concentration. The role of alloy surface morphology and the h-BN growth kinetics will also be discussed.

2D-ThP16 Metal Oxide/Functionalized Graphene Oxide Composite as Highly Stable Lithium Ion Battery Anode with Enhanced Performance, SunSook Lee, Korea Research Institute of Chemical Technology(KRICT), Republic of Korea, *S. Ji, J.Y. Ju, S-K. Kim, J.K. Kim, S. Choi,* Korea Research Institute of Chemical Technology(KRICT)

Metal-oxide based lithium ion battery(LIB) anodes theoretically should provide high specific capacity, but their disappointing experimentally measured capacity and cycle stability inhibit their commercial usage. Here, we propose a simple method to process Metal oxide/functionalized-graphene-oxide(fGO) composite anode, in which fGO is inserted as the current path that simultaneously enhances the specific capacity to reach near the theoretical capacity and the cyclic stability at least up to 200 cycles for the metal oxide based anodes.

2D-ThP18 Exploration of Hybrid 2DEG/Ferroelectric Heterostructure Fabrication Methodology, Stephan Young, E.J. Moon, R. Doucette, A.N. Caruso, University of Missouri - Kansas City

The hybrid two-dimension electron gas (2DEG)/ferroelectric (FE) heterostructure system has many promising applications, including field effect transistors and non-volatile memory. Such devices exploit the ambipolar field effect, utilizing the high local electric field produced by the FE substrate to shift the Fermi level in the 2DEG. Thus, controlling magnitude and direction of polarization of the FE can significantly alter conductivity and majority charge carrier in the 2DEG. FE/2DEG hybrid devices are typically fabricated by transferring the 2DEG onto the FE substrate. However, this process often introduces adsorbates onto the surface of the 2DEG and FE, resulting in a poor interface and degrading the electric field at the 2DEG. This problem can be partially mitigated by improving the transfer process, but direct growth is a path to eliminate the problem entirely. This work explores the effect of different transfer processes in comparison to chemical vapor deposition growth of 2DEG's directly on FE substrates. The study aims to elucidate the interfacial interaction between 2DEG's (i.e. transition metal dichalcogenides and graphene) and low-coercivity, high-remnant-polarization perovskite ferroelectrics. Characterization of the 2DEG domain size was completed with atomic force microscopy, the number of layers confirmed with Raman spectroscopy, and the conductivity of each growth was measured.

This work was supported by the Office of Naval Research (ONR) under N00014-16-1-2067.

2D-ThP20 Effect of Stacking Orientation and Sag on the Strength and Fracture of Graphene Oxide, Teng Cui, C.H. Cao, S. Parambath Mundayodan, Y. Sun, T. Filleter, University of Toronto, Canada

One great challenge in translating the extraordinary mechanical properties of isolated 2D materials to impact real applications is to understand, and bridge the gap, between monolayer and multilayer properties. Bilayer films, as the most fundamental step towards this challenge, require systematic study to unveil the interaction between layers and elucidate the effect on mechanical behavior. Here, bilayer graphene oxide (GO) with different crystalline stacking orientation and sag conditions will be presented, and the resulting effect on the material strength and fracture will be discussed in detail.

Highly oxidized bilayer GO films were prepared on perforated substrates by a solution-based method, from which different interlayer crystalline stacking angle and sagging depth were obtained and characterized. Atomic force microscopy-based mechanical testing revealed higher strength of aligned (small stacking angle) bilayers as compared to misaligned (large stacking angle) counterparts. Further transmission electron microscopy analysis of fracture surface revealed through-film fracture for the aligned case and individual layer cracking for the misaligned case, casting light on the origin of the strength discrepancy. In addition, the suspended GO films present different sagging depth, which in turn is found to effect the load carrying capacity and the fracture behavior significantly. Our results demonstrated that bilayer GO with ~165 nm sag doubles the fracture force as compared to ~ 40 nm sag. A deeper understanding of the configurational effect, e.g., stacking orientation and sagging, on the mechanical behavior will better facilitate engineering GO for various applications at different size scales.

2D-ThP22 Single Atom Manipulation and Controllable Atom by Atom Assembly in 2D Materials via Scanning Transmission Electron Microscopy, Sergei Kalinin, O. Dyck, S. Kim, S. Jesse, Oak Ridge National Laboratory

Fabrication of structure atom-by-atom has remained one of the longest-held dreams of nanoscience, as a key element of nanotechnology and penultimate step for understanding physics and chemistry on the atomic level. The development of scanning tunneling microscopy (STM) in the early 1980s has demonstrated the potential of an atomically sharp tip to induce atomic motion on a surface, originally perceived to be detrimental to microscope operation. The work by Eigler at IBM in the early 1980s demonstrated that tip induced atomic motion can be used for the assembly of functional atomic structures, an accomplishment believed to be one of the key factors that lead to the nanotechnology revolution of the last decades. However, STM operation necessitates low temperature ultra-high vacuum environments and typically results in structures confined to reactive surfaces. Correspondingly, it took over 20 years to transition from atomic manipulation by STM to viable pathways for single-atom devices. This in turn, necessitates the search for alternative methods for single atom manipulation and atom-by-atom assembly.

Here we demonstrate that the sub-atomically focused beam of a scanning transmission electron microscope (STEM) can be used to controllably manipulate individual dopant atoms in a 2D graphene lattice. We demonstrate the manipulation of adsorbed source materials and the graphene lattice with the electron beam such that individual vacancy defects can be controllably passivated by Si substitutional atoms. We further demonstrate that these Si

defects may be directed through the lattice via e-beam control or modified to form new defects which can incorporate new atoms into the graphene lattice. We further explore the application of beam to probe local dynamics within individual or between adjacent atomic sites. These studies demonstrate the potential of STEM for atom-by-atom nanofabrication and fundamental studies of chemical reactions in 2D materials on the atomic level.

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