Friday Morning, November 8, 2024

2D Materials

Room 122 - Session 2D+EM+MN+TF-FrM

2D NEMS and Strain Engineering

Moderators: Susan Fullerton, University of Pittsburgh, **Peter Sutter**, University of Nebraska

8:15am **2D+EM+MN+TF-FrM-1 Engineering the Structure and Properties of 2D Materials by Defects, Strain and Intercalation***, **Arkady Krasheninnikov,*** Helmholtz Zentrum Dresden-Rossendorf, Germany**INVITED**

As 2D materials have a high surface-to-volume ration, nearly all of them contain defects and impurities, which may have appeared due to the effects of the environment or exfoliation, or in case of synthetic materials, during the growth. The defects can govern the electronic and optical properties of 2D systems. Moreover, defects can intentionally be introduced using beams of energetic particles – ions and electrons. Formation of defects may also give rise to phase transformations in these materials and/or tune their properties. Mechanical strain and intercalation by, e.g., alkali metal atoms, can further be used to tailor the materials characteristics. All of these calls upon the studies on defects and their role upon intercalation, response of materials to strain and irradiation. In my talk, I will present the results of our recent theoretical studies of point and line defects in 2D materials [1-4] obtained in close collaboration with several experimental groups. I will further discuss how strain can affect the characteristics of defective 2D materials [5] and how new 2D phases of materials can be created upon atom intercalation between graphene sheets and address the role of defects in this process [6].

1. F. Long et al., Nano Lett. 23 (2023) 8468.

2. F. Davies, K. Mehlich, C. Busse, and A. V. Krasheninnikov, "2D Mater. 11 (2024) 015003.

3. V. Pathirage, et al., Materials Today Nano 22 (2023) 100314.

4. F.H. Davies and A. V. Krasheninnikov, Phys. Rev. B 109 (2024) 165442.

5. P. Santra, et al., npj 2D Materials and Applications 8 (2024) 33.

6. X. Zhang, et al., Mater. Today Ener. 34 (2023) 101293.

8:45am **2D+EM+MN+TF-FrM-3 Band Gap Opening in AB-Stacked Bilayer Silicon***, **Kumar Vishal**, H. Huang, Y. Zhuang,* Wright State University

Despite their potential as of being the excellent candidates for advancing CMOS technology to its physical limits, the presence of an opened energy bandgap in either single- or bilayer- silicene poses a significant challenge, hindering its applications in the main stream semiconductor industry. Previous attempts, including applying external electric field, surface decoration, nanopatterning, and applying uniaxial strain along designate directions, have proven insufficient in meeting the stringent demands of CMOS technology concerning operational reliability, processing environment sensitivity, product yield, and achievable processing standards. Recently a number of research reported that applying of the biaxial in-plane strain leads to energy bandgap opening in AA-stacked bilayer silicene, however the maximum energy bandgap opening is limited to 16 meV.

In this work, we present a theoretical study of the opening of energy bandgap in AB-stacked bilayer silicene. Employing the Density Functional Theory (DFT), our investigations have taken into account of the effects of both ferromagnetism and antiferromagnetism, alongside external biaxial in-plane strain/stress and vertical biasing effects. Within a strain range spanning from -5.17% to 10.35%, we observed a strain-tunable energy bandgap opening with a maximum of 380 meV at a strain level of 7.76%. Notably, beyond this strain range, the energy bandgap remains closed. In addition, under compressive strain, the energy band diagram presents spin-generated features, with discernible energy band splitting. On the contrary, tensile strain leads to a break of the spin generation, except at specific high symmetry points such as Γ, K and M. We further observe a degeneration of the energy band diagram at these high symmetry points upon the application of gate voltage along the vertical direction. The coupling of the ferromagnetism and antiferromagnetism between the two silicene layers results in a transition from metallic material to semiconductor. The potential of the opened bandgap makes the AA-stacked bilayer silicene a very promising candidate material to be applied in the CMOS technology, while the strain-induced tunable bandgap opening offers immediate potential for applications in the infrared (IR) spectrum. In addition, the spin-induced band diagram degeneration may holds promise for integrated spintronics applications.

9:00am **2D+EM+MN+TF-FrM-4 Laser-Induced Strain Tuning in Monolayer Graphene Nanomechanical Resonators***, **Muhammad Ashar Naveed**, S. Pandit, Y. Wang,* University of Nebraska - Lincoln

Graphene, as the paradigm-shifting two-dimensional (2D) material, has demonstrated great potential in micro-/nano-electromechanical systems (MEMS/NEMS) due to its extraordinary mechanical properties, ultimate device thicknesses, and unparalleled flexibility in integration. On the other hand, the atomic thickness and the transfer process employed in device fabrication pose challenges to achieving uniform strain over the entire device. In this work, we utilize Raman spectroscopy and investigate the strain distribution in drumhead resonators based on the mechanically exfoliated graphene monolayers suspended over patterned oxidized silicon (SiO_2/Si) substrates. Moreover, the effects of laser-induced heating and consequential strain tuning have been systematically explored by combining Raman spectroscopy and mechanical resonance measurements. This study sheds light on the strain engineering of monolayer graphene nanomechanical resonators, and the methodology developed is readily applied to other 2D materials and heterostructures.

9:15am **2D+EM+MN+TF-FrM-5 Developing 2D Snse for Piezoelectric Applications***, J. Chin, M. Frye, B. Gardner,* Georgia Institute of Technology*; D. Liu,* Penn State University*; M. Hilse,* Pennsylvania State University*; I. Graham,* Georgia Institute of Technology*; J. Shallenberger, K. Wang, M. Wang, Y. Shin, N. Nayir, A. can Duin, S. Law,* Pennsylvania State University*; **Lauren Garten**,* Georgia Institute of Technology

Unique functionalities can arise when 2D materials are scaled down near the monolayer limit. Tin selenide (SnSe) is one such 2D material which is centrosymmetric in bulk but becomes non-centrosymmetric when reduced to the monolayer limit, enabling piezoelectricity, and potentially, ferroelectricity. Developing 2D piezoelectric and ferroelectric materials is critical for the scaling of efficient sensors and electronics, such as ferroelectric field effect transistors. However, unlike other 2D materials, the strong interlayer bonding makes exfoliating a monolayer of SnSe challenging. Therefore, direct film growth is necessary to control the layer thickness and promote lateral growth large enough for device testing. This talk will focus on the development of processing routes to control the morphology and layering of SnSe thin films grown by molecular beam epitaxy (MBE) for piezoelectric devices. The bulk *Pnma* phase of SnSe is stabilized over a broad range of Sn:Se flux ratios from 250 – 300 °C on (100) MgO and (0001) Al_2O_3 substrates. Changing the flux ratio did not affect the SnSe film stoichiometry; increasing the flux ratio only changes the predominant crystallographic orientation. ReaxFF molecular dynamics (MD) show that the limited stoichiometric change is due to the formation of Se clusters that weakly interact with the surface of the SnSe particles. Changing the temperature, flux ratios, and flux timing had a significant impact on the morphology and orientation of the SnSe thin films. Machine learning was used to infer the critical processing parameters that are needed for creating an oriented, wafer-scale thin film. Overall, this study identifies the conditions for the growth of monolayer SnSe thin films necessary for the development of 2D piezoelectric devices.

9:30am **2D+EM+MN+TF-FrM-6 Two-Dimensional (2D) $FePS_3$ Nanoelectromechanical Resonators with Local-Gate Electrostatic Tuning***, **Yunong Wang**, S. Yousuf, X. Zhang, P. Feng,* University of Florida

Nanoelectromechanical systems (NEMS) based on 2D magnetic materials are promising candidates for exploring ultrasensitive detection and magnetostrictive phenomena due to their high mechanical stiffness, high strength, and low mass. The resonance frequency of the suspended membrane resonator can be probed optically and manipulated mechanically via electrostatically induced strain. This makes electrostatic frequency tuning of the 2D magnetic NEMS resonator a promising way for exploring the novel magneto-mechanical coupling mechanism. Towards building magneto-mechanical coupling NEMS devices, we fabricated circular drumhead $FePS_3$ NEMS resonators with different cavity-diameter sizes (3um to 7um). In this work, we report on experimental demonstrations of high-performance antiferromagnet $FePS_3$ drumhead resonators with the highest frequency tuning range up to 31.62%. We further perform analytical modeling to gain insight and quantitative understanding of the frequency scaling law for $FePS_3$ drumhead resonators. Combining our experimental results and analytical modeling of the resonances, we resolved the elastic behavior of $FePS_3$, including the transition from 'membrane-like' regime to 'plate-like' regime, with built-in tension (γ) ranging from 0.1 to 2N/m. This study not only offers methods for characterizing the mechanical properties of ultrathin membranes of magnetic 2D materials but also provides important guidelines for designing

high-performance magnetic NEMS resonator devices and opens possibilities for building drumhead resonator devices to exploit strain- and dynamics-engineered applications based on ultrathin magnetic 2D crystals.

9:45am **2D+EM+MN+TF-FrM-7 Tunable Phononic Frequency Combs in Atomically Thin Resonators**, ***S M Enamul Hoque Yousuf***, *T. Kaisar,* University of Florida*; J. Lee,* University of Central Florida*; S. Shaw,* Florida Institute of Technology*; P. Feng,* University of Florida

Phononic frequency comb (PnFC), the analogue of optical frequency comb in the radio frequency (RF) regime, has attracted significant research interest due to its potential applications in sensing and computing. In this abstract, we report on PnFCs generation via an atomically thin molybdenum disulfide (MoS_2) nanoelectromechanical resonator. We first measure the nonlinear mode coupling coefficient (λ) due to 1:1 internal resonance from the first-principles approach. To describe the energy exchange between the coupled modes, we employ two resonator equations with a single dispersive coupling term to model the response. The coupled mode equations are solved using the method of averaging to derive a closed form expression for the nonlinear mode coupling coefficient.To calibrate the vibration amplitude of both modes in the displacement domain, we measure the undriven thermomechanical noise.The nonlinear shift of the resonance frequency of mode 1 (f_1) that results from the dispersive coupling to mode 2 is measured as we drive mode 2 near its natural frequency (f_2). We estimate the mode coupling coefficient using our derived model.Additionally, we investigate the impact of Duffing nonlinearity on the energy cycling of the modes.

We utilize the 1:1 internal resonance to couple energy between two modes. The resonator response can be tuned from stable periodic response to quasi-periodic response by controlling external perturbation signals, such as DC gate voltage, RF drive voltage and frequency. The resonator exhibits three unique comb regions with well-defined comb structure. We observe that the periodic and quasiperiodic branches exist for a particular drive voltage and frequency, based on distinct initial conditions. Our demonstration leads the way to achieving tunable PnFCs in nanoscale devices to study nonlinear modal interactions and build ultrasensitive sensors and computing devices.

10:00am **2D+EM+MN+TF-FrM-8 Longitudinal Sound Speed Determination in 2D Semiconducting Crystal of GaS by Broadband Time-Domain Brillouin Scattering**, ***Watheq Al-Basheer***, King Fahd University of Petroleum & Minerals, Saudi Arabia*; C. Viernes, R. Zheng, S. Netzke, K. Pichugin, G. Sciaini,* University of Waterloo, Canada

Due to their unique structure and exceptional physicochemical characteristics, 2D semiconducting materials like GaS have recently attracted significant interest, making them viable options for numerous photonic industries and applications. In this study, time-domain broadband Brillouin scattering measurements were performed on a single, flake-like gallium sulfide (GaS) crystal to determine the out-of-plane longitudinal sound speed, evaluated at (3140 ± 20) m/s. As a member of the group-III monochalcogenide semiconductors, GaS has recently attracted significant attention owing to its remarkable semiconducting properties.Moreover, its high absorption coefficient and efficient carrier mobility have made it a perfect candidate in many photonic and optoelectronic applications and industries, such as fast UV photodetectors,hydrogen evolution catalysis, field-effect transistors,energy storage, gas sensing, and nonlinear optics. The reported results demonstrate the effectiveness of this non-destructive, all-optical technique for investigating the elastic properties of fragile 2D layered materials and provide the value of the out-of-plane compressive elastic constant,

Keywords

Time-domain Brillouin scattering, coherent acoustic phonons, broadband transient spectroscopy,

elastic constant, sound speed, 2D semiconductors, GaS, layered materials.

Author Index

Bold page numbers indicate presenter