

Thursday Afternoon Poster Sessions, November 10, 2016

2D Materials Focus Topic

Room Hall D - Session 2D-ThP

2D Materials Poster Session

2D-ThP1 Vacuum Properties and Operation Stability of the RFQ Accelerator in J-PARC Linac, Takatoshi Morishita, Japan Atomic Energy Agency, Japan

The J-PARC accelerator comprises an injector linac, a 3-GeV Rapid-Cycling Synchrotron and a 50-GeV Main Ring. The beam energy of the linac has been upgraded from 181 MeV to 400 MeV in 2013. For the beam current upgrade, the new frontend (RF ion source, RFQ, chopping system) has been installed for 1 MW operation at RCS. The new RFQ, which is designed for 50 mA beam acceleration from 0.05 MeV to 3 MeV, has been high-power tested and beam acceleration tested at the test station before the installation. The existing RFQ, which is 30 mA design, was replaced to 50 mA RFQ in the accelerator tunnel in summer 2014. After two weeks vacuum pumping, the high-power RF conditioning has been started in the middle of September, then, the user operation started in the beginning of November, 2014. Since then, the RFQ operates without serious problems for more than one year, however, the operation stability with beam acceleration was not enough due to the sparking in the RFQ cavity. We consider that the impurities in the vacuum chamber are related to this sparking phenomena. In this paper, the relation between the sparking rates, the residual gas species in the cavity, beam operation parameters are described.

2D-ThP2 Inkjet Printing Of Liquid-Exfoliated, Highly Conducting Graphene Nanosheets, J. Desai, M. Michel, C. Biswas, R. Hossain, Jorge Catalan, A.B. Kaul, University of Texas at El Paso

Graphene consisting of just one sheet of carbon atoms arranged in a honeycomb lattice is a thinnest two-dimensional (2-D) material known since its discovery in 2004. It finds applications in printed electronics, flexible displays, fuel cells, solar cells and range of other applications due to its high strength and good thermal and electrical properties. Two-dimensional materials are formed from layered materials which can be defined as materials having strong in-plane covalent bonding but weak out-of-plane van der Waals bonding. Exfoliation, i.e., shearing of individual monolayers of layered materials to get two-dimensional materials, can lead to breakage of van der Waals bonding and production of thin atomic two-dimensional nanosheets. Liquid-phase exfoliation refers to exfoliation in suitable solvents. It is a versatile, scalable and sustainable route for production of 2-D nanosheets. Inkjet printing is a material-conserving deposition technique used for printing patterns and devices using liquid-phase materials. The present challenges in printed electronics include finding an appropriate common solvent for exfoliation and printing, printing highly conductive and uniform graphene patterns, preventing nozzle clogging and non-uniform spread of ink on substrate, promoting adsorption and preventing absorption of inks. In our work, we demonstrate highly conductive graphene patterns produced by liquid-phase exfoliation of layered graphite in N-Methyl-2-pyrrolidone (NMP) followed by inkjet printing. We have found an avenue to tailor the viscosity of NMP through the addition of PEDOT: PSS or Poly (3,4 ethylenedioxythiophene)-poly(styrenesulfonate), making it suitable for inkjet printing. Our ink jet printed dispersions show a uniform microstructure, good optical absorbance values and higher concentration of graphene in our final exfoliated solvent using the novel techniques we have developed.

2D-ThP3 Electronic Transport Properties of Hybrid Graphene-C60 Structures, S. Chugh, C. Biswas, Avra S. Bandopadhyay, G. Lara, L. Echegoyen, A.B. Kaul, University of Texas at El Paso

Since graphene was first mechanically exfoliated in 2004 using scotch tape [1], it has attracted intense interest due to its unique electrical, mechanical and thermal properties. Since then, rapid advances have been made in the large-area deposition of graphene films and its ensuing applications. At the same time, C₆₀ fullerenes and their derivative structures also display remarkable chemical reactivity [2]. Various hybrid materials created by organic functionalization of fullerenes have generated intense attention, driven by the possibility of combining some of the outstanding properties of these zero-dimensional materials with those of higher order dimensionality [3]. In this work, we report on the electrophoretic deposition of C₆₀ on the graphene. The synthesized graphene films were characterized using Raman spectroscopy and Scanning Electron Microscopy (SEM), and electrical contacts were made to the graphene flakes of varying sizes using a lift-off process. Then, C₆₀ was synthesized and deposited via an electrophoretic deposition technique. Electronic characterization of the

structures was conducted before and after the attachment of C₆₀ over a wide range of temperatures. A comparative study was made to analyze the resistivity and conductivity as a result of the interaction with the Si/SiO₂ substrate. Also, we discuss the potential application of graphene based C₆₀ structures as flexible transparent electrodes in photovoltaic devices.

Keywords: Graphene, CVD, Raman Spectroscopy, SEM, electrophoretic deposition, C₆₀

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[2]Dirk M, Acc. Chem. Res., 33 (10), 695-703 (2000).

[3] Dingshan Yu, J. Phys. Chem. Lett., 2 (10), 1113-1118 (2011).

2D-ThP4 Comparative Study of the Optical and Electrical Properties of Fluorine-doped Tin Oxide Films Obtained by Spray Pyrolysis Techniques, Karim Monfil-Leyva, R.C. Ambrosio-Lázaro, J.A. Luna-López, Benemerita Universidad Autónoma de Puebla, Mexico; A.L. Muñoz-Zurita, Universidad Politécnica Metropolitana de Puebla, Mexico

Research and development of Transparent Conducting Oxides (TCOs) has increased due to their many industrial applications. In particular, Fluorine doped Tin Oxide (FTO) is actually needed to develop semiconductor devices because this material has repeatable optical and electrical properties. This work shows a comparative study of the optical and electrical properties of FTO thin films obtained by electronic spray pyrolysis and ultrasonic spray pyrolysis techniques. A chemical solution for spraying purposes was prepared with stannic chloride (SnCl₄) dissolved in ethanol (C₂H₆O₂) mixed with ammonium fluoride (NH₄F). FTO thin films were deposited on glass substrates varying the distance from the nozzle to the hot plate. Spray pyrolysis system was controlled by an electronic trigger. Ultrasonic pyrolysis system was controlled by a resonant frequency. The transmittance and reflection properties were measured using an UV-Vis Spectrophotometer and the band gap energy was determined. The average transmittance in the visible range of FTO films was even above 85%. All FTO films were characterized using X-Ray Diffraction (XRD) and Scanning Electron Microscopy (SEM). The X-ray diffraction patterns showed that main growth orientations were [110], [101] and [211]. SEM images showed homogeneous surface on FTO films but they also indicated a change on nano-cluster sizes and density according to the distance from the nozzle to the hot plate and according to the used spray pyrolysis technique. XRD results were used to calculate the grain size and lattice parameters. The chemical composition of the FTO films was also analyzed using Electron Diffraction Scanning (EDS) and the obtained atomic concentration was compared. Sheet resistance was measured using a four points arrangement and the minimum sheet resistance was 14 Ω/square. Optical and electrical results of the FTO thin films showed suitable properties for photovoltaic and optoelectronic applications using fast, cheap and large area deposition techniques.

2D-ThP5 Selective Molecular attachment for 3D Printing of 2D Circuits, A.T. Juhl, N.R. Glavin, G.M. Leuty, R.J. Berry, R.R. Nair, M.F. Durstock, E.M. Heckman, R.S. Aga, E.B. Kreitz, Air Force Research Laboratory; Wenbi Lai, C. Muratore, University of Dayton

Recently, we utilized phage display techniques to identify peptides that selectively bind to 2D targets such as electrically conductive graphene and semiconducting MoS₂ in the forms of micro-scale fine powder, bulk crystals, and ultra-thin films (<1.5-5 nm). To examine the nature of peptide binding to these materials, we produced different 'inks' comprised of peptide molecules known to selectively bind to each material in solvents for printing on diverse surfaces including SiO₂, gold, and PDMS. Each ink only binds to one type of particle (graphene or MoS₂). We then exposed the substrates printed with peptides to suspensions of 2D particles. The particles demonstrate strong binding to the printed peptide surfaces, demonstrating a new scalable technique for large area device fabrication from 2D materials on diverse surfaces. To further understand peptide-MoS₂ surface binding mechanisms, molecular dynamics simulations employing a newly developed atomic force field predicting the surface energy of MoS₂ films were conducted. Integration of binding peptides into the model in conjunction with experimental results promote fundamental understanding of molecular interactions with MoS₂ and other TMD materials for development of novel sensors and devices.

2D-ThP6 Image Potential State of Graphene on Iridium Modulated by Oxygen Dosing, Yi Lin, Y.Z. Li, J. Dadap, R. Osgood, Columbia University

Image potential state are an important class of surface states, which can be used to probe the chemical and structural properties of metallic or dielectric crystals. Recently the existence of image states has been reported for graphene and graphene on metal such as the Fauster and

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Osgood, Hoefer, and Petek Groups. However, understanding of the effects of adsorbates on Gr surfaces has not been extensively studied either theoretically or experimentally. An important issue is the change of the electronic structure of the image potential states at graphene-metal interface due to oxygen absorption. Thus we have recently carried out the study on the image potential system for graphene on iridium (111) as altered by oxygen dosing.

The epitaxial graphene on iridium is prepared by repeated cycles of temperature programmed growth (room-temperature ethene exposure 2×10^{-5} torr for 45 s and then flashing to 1450 K. This procedure is known to lead to self-limited growth such that exactly one graphene monolayer are formed on the single crystal Iridium substrate (*in situ* cleaned by many annealing and sputtering cycles). The oxygen adsorption is done simply by pure oxygen gas injection by 10^{-5} Torr. The cleanness of the iridium substrate, the growth of monolayer graphene on iridium and the absorption of oxygen are monitored by *in situ* low energy electron diffraction (LEED) patterns. Our 2PPE experiments are conducted using either monochromatic or bichromatic femtosecond pulses with the pump photon energy generally in the 4.2 eV range. An optical parametric amplifier, driven by 250 kHz Ti-sapphire laser, generates tunable laser pulses from 1.5-6.1 eV, pulse duration 90 fs and pulse energy 1 nJ. Photoemission electrons are detected along the M-G-M direction of the Brillouin zone using a spherical-sector energy analyzer with 50 meV energy resolution. Care is taken to prevent distortion of the photo-emitted electron energy distribution by space charge effects.

With this instrument, the state energy, its dispersion and the decay time of the first image potential states of the oxygen-absorbed graphene on iridium are measured. We compare our results of oxygen-dosed graphene on iridium with previous reported results of pure graphene on iridium. The shift of the states, the broadening of the dispersion and the change of the dynamic process are modeled and discussed, which provides new insight on using image states for surface probing, as well as the effects of dosing on image state physics.

This work was supported by the Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award Contract No. DE-FG 02-04-ER-46157.

2D-ThP7 Raman Spectroscopy and Optical Characterization of Thermoelectric Devices From Ni/Bi₂Te₃/Sb₂Te₃/Ni Thin Films, Aschalew Kassu, S. Budak, Z. Xiao, R. Hammond, X. Crutcher, A. Sharma, Alabama A&M University

Thermoelectric devices from Ni/Bi₂Te₃/Sb₂Te₃/Ni thin films were prepared. The thin films are deposited by using DC/RF magnetron sputtering and E-beam deposition systems. The surface morphology of the fabricated thermoelectric films is characterized using Scanning Electron Microscope (SEM). Raman spectroscopic technique is used for identification of inherent molecular specificity and analysis of chemical compositions of the films. The resonant features of the scattering spectra measured under the 532 nm and 785 nm wavelength excitation lasers are analyzed.

Acknowledgement

This research was supported by NSF with grant numbers NSF-HBCU-RISE-1546965, NSF-EPSCOR-R-II-3-EPS-1158862, DOD with grant numbers W911 NF-08-1-0425, and Department of Homeland Security-Scientific Leadership Award, Grant No. DHS-SLA 2014-ST-062-000060

2D-ThP8 Thermoelectric Generators from SiO₂/SiO₂+Au Thin Films For Energy Harvesting, S. Budak, Z. Xiao, M. Curley, Justin Cole, C. Birchfield, M. Howard, B. Rodgers, T. Strong, Alabama A&M University

Thermoelectric generators were prepared from multilayered SiO₂/SiO₂+Au thin films using DC/RF magnetron sputtering system. Thermoelectric devices were annealed at different temperatures to form nanostructures in the multilayer thin films to increase the Seebeck coefficients and electrical conductivity and decrease thermal conductivity. The prepared devices were characterized using Seebeck coefficient measurement; four probe van der Pauw measurement resistivity and the laser thermal conductivity systems. The surface morphology of the fabricated thermoelectric films is characterized using Scanning Electron Microscope (SEM+EDS). TE devices will also be characterized as if they are wave-guides. Mode index, propagation loss, refractive index profile with respect to the dose, depth of the thin films will be analyzed as a function of annealing temperatures.

Acknowledgement

Research was sponsored by NSF with grant numbers NSF-HBCU-RISE-1546965, NSF-EPSCOR-R-II-3-EPS-1158862, DOD with grant numbers W911

NF-08-1-0425, and W911NF-12-1-0063, U.S. Department of Energy National Nuclear Security Administration (DOE-NNSA) with grant numbers DE-NA0001896 and DE-NA0002687.

2D-ThP9 Advanced Thermoelectric Devices from Ni/Bi₂Te₃/Sb₂Te₃/Ni Thin Films for Energy Harvesting, S. Budak, Z. Xiao, M. Curley, Cody Birchfield, J. Cole, M. Howard, B. Rodgers, T. Strong, Alabama A&M University

Thermoelectric devices were prepared from Ni/Bi₂Te₃/Sb₂Te₃/Ni thin films using E-beam deposition and DC/RF magnetron sputtering systems. Fabricated devices were annealed at different temperatures to form nanostructures in the multilayer thin films to increase both the Seebeck coefficients and electrical conductivity and decrease thermal conductivity. The thermoelectric devices were characterized using Seebeck coefficient measurement system; four probe van der Pauw measurement resistivity system and the laser thermal conductivity system. The surface morphology of the fabricated thermoelectric films is characterized using Scanning Electron Microscope (SEM). TE devices will also be characterized as if they are wave-guides. Mode index, propagation loss, refractive index profile with respect to the dose, depth of the thin films will be analyzed as a function of annealing temperatures.

Acknowledgement

Research was sponsored by NSF with grant numbers NSF-HBCU-RISE-1546965, NSF-EPSCOR-R-II-3-EPS-1158862, DOD with grant numbers W911 NF-08-1-0425, and W911NF-12-1-0063, U.S. Department of Energy National Nuclear Security Administration (DOE-NNSA) with grant numbers DE-NA0001896 and DE-NA0002687.

2D-ThP10 VUV-photoassisted Chemical Doping on Graphene Oxide, Masahiro Soga, Y. Tu, T. Utsunomiya, T. Ichii, H. Sugimura, Kyoto University, Japan

Chemical doping on graphene and its derivatives is a powerful technique for modulating their electronic properties¹. Especially, nitrogen doping can help the electron transfer and enhance the electrocatalytic activity. Nitrogen doped graphene have been synthesized by thermal annealing approach and hydrothermal reduction of graphene oxide (GO) in the presence of N₂H₄ and NH₃ in general^{1,2}. However, these methods are high cost, complicated and suffer from toxic chemicals. In this research, nitrogen doped and reduced graphene oxide (N-rGO) was synthesized by vacuum ultraviolet (VUV) irradiation.

Colloidal dispersion of GO sheets was prepared by the modified Hummers' method. NH₃ aqueous solution (14.8 M) was added to the GO dispersion and was magnetically stirred for 24 hours. After that, the dispersion was centrifuged at 13.5 krpm for 10 min and washed ten times with ultra pure water, and then aqueous dispersion of nitrogen modified GO (N-GO) was obtained. The N-GO dispersion was spincoated on Si substrate and VUV light ($\lambda = 172$ nm, 10 mW cm⁻²) was irradiated on this sample under high vacuum condition ($< 10^{-3}$ Pa) for 64 min. The sample was characterized by Fourier transform infrared spectroscopy (FT-IR) and X-ray photoelectron spectroscopy (XPS).

XPS and FT-IR analysis of the samples revealed that chemically reactive oxygen functional groups in a GO sheet reacted with ammonia and the formation of C-N bond proceeded after stirring in NH₃ aqueous solution. After VUV irradiation, XPS and FT-IR analysis showed that N-GO was reduced and bonding configuration of nitrogen was changed.

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2. D. Long, W. Li, J. Miyawaki, I. Mochida, S. Yoon, Langmuir 26, 16096 (2010)

2D-ThP11 Tungsten Diselenide Nanoribbons Formed by Focused Helium Ion Beam Induced Etching, Michael G. Stanford, P.R. Pudasaini, A.T. Wong, A. Hoffman, D.G. Mandrus, P.D. Rack, The University of Tennessee Knoxville

The helium ion microscope (HIM) has garnered much attention in recent years due to its high resolution and precision as a nanoprocessing tool. In this work, we introduce a focused helium ion beam induced etching (FIBIE) process which enables direct-write patterning of WSe₂. The etching process utilizes the XeF₂ precursor molecule to provide a chemical etch assist for rapid material removal. The FIBIE process enables the high fidelity patterning of WSe₂ with He⁺ doses an order of magnitude lower than standard He⁺ milling procedures. Of particular interest, transition metal dichalcogenide (TMD) nanoribbons exhibit unique magnetic properties depending upon edge termination. However, few experimental studies have been conducted on TMD nanoribbons due to difficulty of fabrication.

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The FIBIE process enables the straightforward direct-write fabrication of aligned arrays of WSe₂ nanoribbons with dimensions as low as 8 nm. The WSe₂ nanoribbons demonstrate high optical anisotropy and electrical measurements are reported for the first time. We also study the magnetic properties and report magnetoresistance of devices fabricated from WSe₂ nanoribbon arrays.

2D-ThP12 Tuning the Electronic Structure of Metallic Single Crystal Surfaces through Ultra Thin Hetero-Junctions for Photocathode Applications, ZhengRong Lee, R. Seibert, D. Velázquez, L. Spentzouris, J. Terry, Illinois Institute of Technology

The development of photocathodes for the next generation of state-of-the-art laser-driven photoinjectors requires the use of photoemissive materials with specific characteristics depending upon their application (FELs, ERLs, Wakefield acceleration, etc.). The ability to tune the emissive properties of photocathodes to match the requirements of the specific accelerator device could have a important impact in research and development. In this work we show that such photoemissive tunability can be achieved through the engineering of single crystal metallic surfaces by coating them with metal-insulator heterojunctions of various thicknesses. Ultrathin multilayered MgO/Ag(001)/MgO films were grown by pulsed laser deposition, tuning the thickness n of the flanking MgO layers to 0, 2, 3, and 4 monolayers. We observed an increase in quantum efficiency and simultaneous decrease in work function with layer thickness. The scale and trend direction of measurements are in good but not excellent agreement with theory. Angle resolved photoemission data for the multilayered sample $n = 3$ showed that the emission profile has a metallic-like momentum dispersion. Deviations from theoretical predictions [K. Németh et al., PRL 104, 046801 (2010)] are attributed to imperfections of real surfaces in contrast with the ideal surfaces of the calculation.

2D-ThP13 Electronic Structure of Bulk WSe₂ and Multilayer WS₂, Iori Tanabe, University of Nebraska-Lincoln; *T. Komesu,* University of Nebraska - Lincoln; *E.F. Schwier,* Hiroshima Synchrotron Radiation Center; *M. Gomez, L. Bartels,* University of California - Riverside; *M. Zheng, Y. Kojima,* Hiroshima University; *E.M. Echeverria,* University of Nebraska-Lincoln; *A.V. Barinov, S.K. Baliapalli, V. Kandyba,* Elettra - Sincrotrone Trieste; *K. Shimada,* Hiroshima Synchrotron Radiation Center; *P.A. Dowben,* University of Nebraska - Lincoln

WSe₂ and WS₂ and the related transition metal dichalcogenides (TMDs) MX₂ (with M = V, Mo, W, Ta and X = S, Se, Te) are layered structures, where each plane consists of a hexagonal honeycomb lattice reminiscent of graphene or graphite. The distinguishing features of TMDs compared to graphene are that TMDs are semiconductors and TMDs monolayers have C_{3v} symmetry, not C_{6v} symmetry, since the metal and chalcogen planes are offset from each other. We investigated the valence band structure of bulk WSe₂ and multilayer WS₂ using angle resolved photoemission spectroscopy (ARPES). These ARPES studies of the electronic band structure of bulk WSe₂ and multilayer WS₂ provide a means to compare the effective hole mass and the splitting of the top of the valence band at K, due to spin-orbit coupling for various transition metal dichalcogenides. The splitting of the top of the valence band at K was measured to be 0.49±0.01 eV and 0.42±0.03 eV, for bulk WSe₂ and multilayer WS₂ respectively. In both cases, the splitting due to spin orbit coupling are far larger than that for MoS₂, but smaller than that for monolayer WSe₂. We found that the effective mass at the top of the valence band at K of WSe₂ and WS₂ were very small, which indicates very high intrinsic mobility and is consistent with expectations from density functional theory. The electron effective masses, as derived from angle-resolved inverse photoemission, are found to be much greater than anticipated.

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