6th PREM ANNUAL MEETING
November 20, 2009
Palmas de Mar, Humacao P.R.

9:15 - 10:00 AM **Registration & Breakfast**

10:00 - 10:10 AM **Welcome Messages**
Idalia Ramos, PREM PI
Aida Rodríguez Roig, UPRH Academic Dean
Andrew McGhie, Associate Director PENN MRSEC
Arjun Yodh, PREM Co-PI, Director PENN MRSEC

10:10 - 10:40 AM **Overview of New PREM Grant**
Idalia Ramos, **Andrew McGhie** and **Arjun Yodh**

10:40 - 11:10 AM ***Reinforced elastomers at large strains: Effective behavior, microstructure evolution and macroscopic instabilities***
Pedro Ponte, UPENN

11:10 - 11:30 AM ***Cavitations and wrinkling instabilities for solids***
Pablo Negrón, UPR-Humacao

11:30 - 11:50 PM ***Fabrication of biodegradable scaffolds for biomedical applications***
Víctor Pantojas, UPR-Cayey

11:50 - 12:10 PM **Biosensing approaches toward the detection of pathogens**
Ana Guadalupe, UPR-Río Piedras

12:10 - 1:30 PM **Working Lunch**

1:30 - 1:50 PM ***Diodes fabricated from electrospun nanofibers of organic/inorganic materials*, Nicholas Pinto**, UPR-Humacao

1:50 - 2:10 PM ***Gallium Nitride nanofibers fabricated by electrospinning***
Idalia Ramos, UPR-Humacao

2:10 - 2:30 PM ***Graphene based superlattice***
Raphael Tsu, University of North Carolina, Charlotte

2:30 - 2:50 PM ***Nano Opto-Mechanical Systems NOMS*, Eva Campo**, Lehigh University

2:50 - 3:00 PM **Posters Setup**

3:00 - 4:30 PM **Students Posters Presentations**

4:30 - 5:30 PM **Advisory Committee meets to write Report**

5:30 PM **Closing**

Faculty Research Presentations

Reinforced elastomers at large strains: Effective behavior, microstructure evolution and macroscopic instabilities

Pedro Ponte
UPENN

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In this talk I will present applications of the "variational linear comparison" nonlinear homogenization technique to generate estimates for the effective behavior, microstructure evolution and loss of ellipticity in reinforced elastomers at finite strains. Three special cases will be considered for illustrative purposes: short-fiber composite elastomers, long-fiber reinforced rubbers and thermoplastic elastomers (TPEs). In particular, for the short-fiber composites, we investigate the rotation of the rigid particles in the context of finite elasticity, and make comparisons with Jeffery's solution for rigid particles in a Newtonian fluid. For the long-fiber composites, we make comparisons with Rosen's estimates for the possible development of instabilities (using a two-dimensional laminate model). For the TPEs, which are block copolymer systems with a hard glassy phase serving to provide reinforcement in a softer rubbery matrix phase, we explore the effect of structure at two different length scales: a lamellar structure at the nanometer scale and a granular structure at the micrometer scale. In all these material systems, it is found that even when the constituent phases are strongly elliptic, their overall behavior may lose ellipticity at sufficiently large deformations, corresponding to the possible development of shear band-type instabilities. The source of these "macroscopic" instabilities has been identified with the evolution of the microstructure, which, under appropriate loading conditions, can induce "geometric softening" leading to the overall loss of ellipticity.

Cavitations and wrinkling instabilities for solids

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Pablo Negrón
UPR-Humacao

Errol Montes-Pizarro, University of Puerto Rico- Cayey
Jey Sivaloganathan, University of Bath, UK
Pedro Ponte-Catañeda, University of Pennsylvania

In this talk we discuss some numerical and theoretical results for the characterization of material instabilities in solids of either cavitation or wrinkling type. To describe these sort of phenomena we employ a model of nonlinear elasticity, which is more appropriate due to the large stresses (potentially infinite) associated with the large compressions or expansions involved in such deformations. For the problem of cavitation we give a new characterization of the type of deformations producing holes inside a body which originally had no holes, i.e., no imperfections. We discuss how this characterization might lead to a numerical procedure for computing these critical hole producing three dimensional deformations for a given specific material.

To study wrinkling instabilities we use a tool from the theory of partial differential equations called the complementing condition. For deformations of cylindrical structures and for a general class of materials (Green-Hadamard) we show that failure of the complementing condition is directly associated with a wrinkling type instability. Failure of the complementing condition is equivalent to a certain algebraic equation having solutions, thus leading to a numerical procedure for checking whether or not wrinkling instabilities are possible for a specific material.

As the materials normally used in engineering applications are composites, i.e., mixtures of other basic materials, we study the characterization of material instabilities, like cavitation or wrinkling, for composite materials. For simplified version of this problem using a nonlinear Poisson type equation, we present some simulations that resemble composite materials with voids (empty inclusions) and with (filled) inclusions.

Fabrication of biodegradable scaffolds for biomedical applications

Victor Pantojas
UPR-Cayey

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Scaffolds composed of a mixture of polylactic acid (PLLA) and Polyethylene Glycol (PEG) biodegradable polymers were prepared by electrospinning. Three-dimensional scaffolds of highly porous non-woven fibers were produced and coated with hydroxyapatite for bone tissue engineering. A mixture (80/20) of PLLA/PEG was dissolved at 5.7 %, 7%, 8% and 9% blend solution concentration. The structure and morphology of the scaffolds were investigated by scanning electron microscopy. Fiber diameters ranging from 250 nm to 2 μm were obtained as a result of the change in viscosity. For samples deposited at 9% concentration, individual fibers contain pores with nanometric dimensions. For applications in bone formation, recent efforts on coating the scaffold's fibers with hydroxyapatite, the ceramic constituent of bone, are described. The crystallinity of the hydroxyapatite coating deposited by sputtering was evaluated by x-ray diffraction. The coatings were found to be mostly amorphous.

Biosensing approaches toward the detection of pathogens

Ana Guadalupe
UPR-Río Piedras

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During the new PREM grant period we continue our efforts toward the optimization of an electrochemical platform for the detection of nucleic acids (probe-target) hybridization. A Nucleic Acid Biosensor is being developed using a polymer modified electrode surface together with an electroactive ferrocene (Fc) derivative. To test this prototype, Salmonella is used as the target microorganism. Polystyrene (PS) films functionalized with nucleic acid sequences (probes) from the Salmonella genome are used to modify carbon electrode surfaces. The hybridization step is detected by looking at the Fc redox process in various schemes. A Fc label and a water soluble Fc-PEG derivative are used to design different detection strategies. The goal is to choose the configuration that affords the best response without the need for target modification. Several PS films and anchored nucleic acid sequences with different lengths at gold and carbon surfaces have been synthesized.

Diodes fabricated from electrospun nanofibers of organic/inorganic materials

Nicholas Pinto
UPR-Humacao

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Electrospinning has been the primary use in our group for the fabrication of polymer nanofibers. This is a simple technique that is very economical and leads to the production of long (several cm) nanofibers. We have used this method to prepare nanofibers of various polymers and ceramic oxides. One of our research projects focused on the fabrication of *p-n* and Schottky diodes and their electrical characterization. Typically, such diodes were fabricated using spin coating techniques and were 2-D in nature with the active region covered with electrodes. In the case of our diodes which are quasi 1-D, in addition to being rectifiers under ambient illumination or in the dark, the advantage of our design is the complete exposure of the rectifying nano-junction to the surrounding environment, making them attractive candidates in the potential fabrication of low power consumption diodes and rapid response sensors. This talk will focus on our research accomplishments during the last year.

Gallium Nitride nanofibers fabricated by electrospinning

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Idalia Ramos
UPR-Humacao

Anamaris Meléndez and Kristle Morales, University of Puerto Rico-Humacao
Eva Campo, Lehigh University
Jorge J. Santiago-Avilés, University of Pennsylvania

Gallium Nitride (GaN) nanostructures have important characteristics for optoelectronics and gas sensing applications. GaN nanofibers have been produced using electrospinning and a precursor solution composed of a mixture of Gallium (III) Nitrate Hydrate dissolved in Dimethyl-Acetamide (DMA) and a viscous solution composed of Cellulose Acetate dissolved in Acetone and DMA. The resulting electrospun nanofibers fibers were sintered at 400°C in Nitrogen for one hour to decompose the polymer. Then, the furnace atmosphere was switched to NH_3. The fibers were sintered for periods of 3, 5 and 7 hours at 900°C under a NH_3 gas flow. The properties of the fibers produced using this method have been studied using X-ray Diffraction (XRD), Environmental Scanning Electron Microscopy (ESEM), Transmission Electron Microscopy (TEM), Fourier-Transform Infrared Spectroscopy (FTIR) and Ultraviolet-Visible Spectroscopy (UV-Vis). Results show the production of GaN nanofibers with hexagonal wurtzite structure. The I-V characteristics of single nanofibers show increments in conductivity for the fibers ammoniated for longer periods of time. Experiments have been conducted using UPR-Humacao, PENN and Lehigh University facilities. Current efforts aim at improving the fabrication process and to conduct sensing and photoluminescence tests.

Graphene based superlattice

Raphael Tsu
University of North Carolina, Charlotte

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The original superlattice involves man-made periodic structures for the purpose of tailoring size to fit the best device configuration. The coherent electronic property such as Bloch oscillation due to Bragg refraction at the Brillouin Zone boundary forms the foundation of THz oscillators and amplifiers. Recently, the field of Bucky Ball and Carbon Nano-tube has evolved into hot activities involving the SP^2 2D graphene with bonds stronger than diamond. In 1982, I was involved in discovering that coal is basically intercalated graphite with aluminates and silicates. On heating between 600 – 700C, the conductivity increases from almost insulating to something within a factor of five from graphite. This brought to some new ideas of superlattice, by relaxing the coherence of individual components, and paying more attention on symmetry and ordering in the structural packing. Instead of going for THz devices, we want to drastically broaden the functionality of man-made materials, trading coherency with packing arrangement. For example, packing quantum dots and quantum wires into a composite to control shapes and its relationship to voids may result in a new kind of incoherent composites with special functions such as nonlinear optical properties, and mechanical features such as the elastic and piezoelectric properties. The main difference from the graphite intercalation lies in the manner we proceed to pack something in between graphene sheets using MBE or CVD deposition techniques. The broad procedure involves wrapping something with graphene sheets.

Nano Opto-Mechanical Systems NOMS

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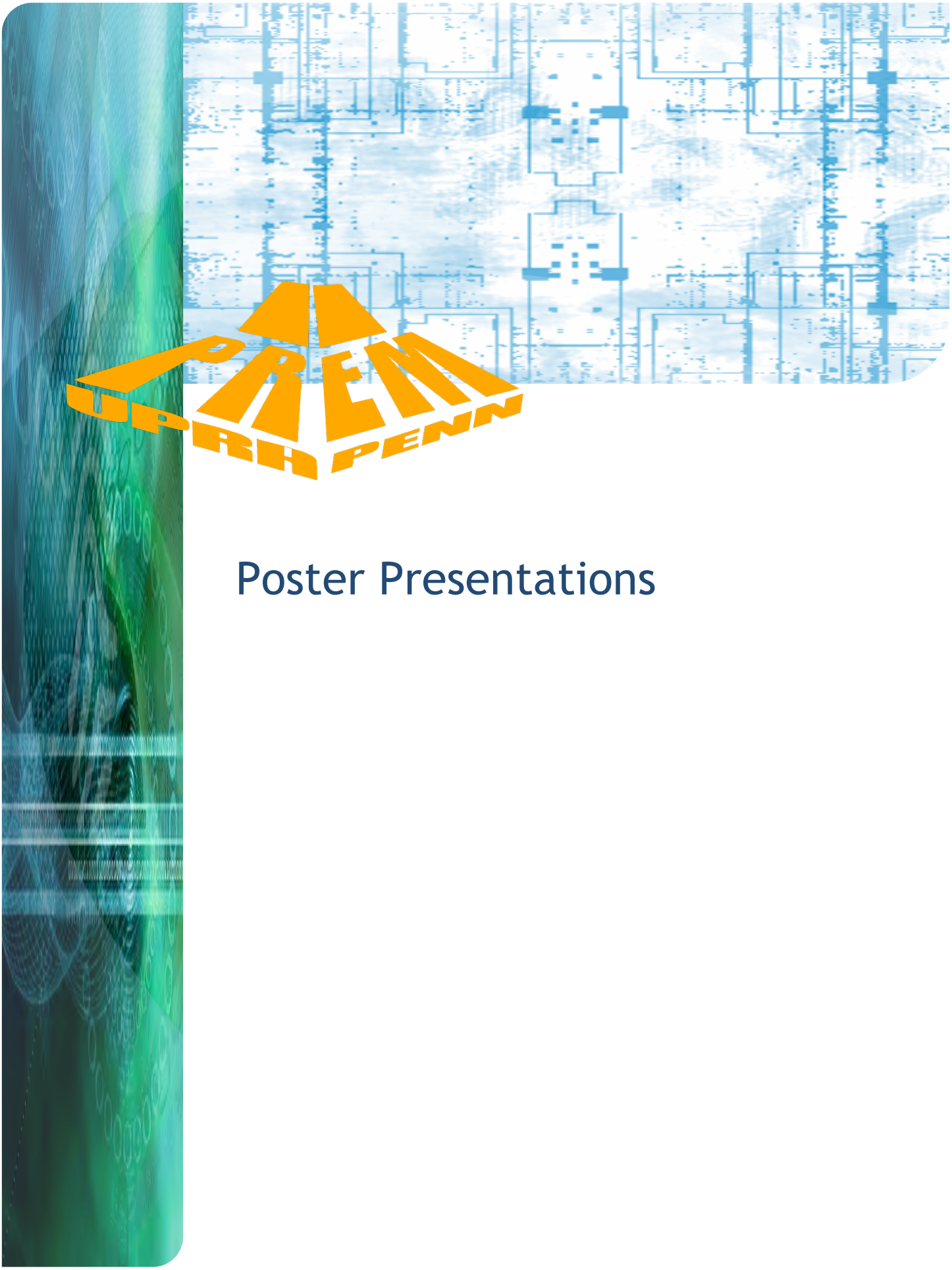
Eva Campo
Lehigh University

Humberto Campanell, Jaume Esteve and José A. Plaza, Instituto de Microelectrónica de Barcelona (IMB-CNM)
Jordi Roig, Universitat Autònoma de Barcelona
Igor Krupa and Maria Omastova, Ustav Polymerov, Slovenska Akademia Vied, Slovakia
Eugene M. Terentjec, University of Cambridge, UK
Branislav Mamojka, Slovak Blind Union
Brigitte Roder, University of Hamburg
David Wenn, IxScient

Nano-opto mechanical Systems (NOMS) based on the photoactuation of optoactive polymer actuators and devices (OAPAD) is a much sought-after technology. In this scheme, light sources promote mechanical actuation of polymeric materials producing a variety of nano–opto mechanical systems such as nano-grippers. The European Union NOMS consortium is a multidisciplinary team assembled to build a tactile tablet for the visually-impaired. The consortium is formed by experts in materials, optics, microsystems, neuropsychology, as well as end users, and commercial partners who will fabricate the first visual aid tablet based on photoactuation technology.

The purpose of this paper is to stir an interest in the field of photoactuators; promoting OAPAD to mainstream R&D. To this purpose, we will review the current state of the art on photoactuators and address outstanding concerns towards microsystem integration. Photoactive actuators could be a complement to Electroactive Polymer Actuators and Devices (EAPAD). Indeed, the “wireless” character of optical actuation could pose an advantage to electrical actuation in some environments. Albeit, given the similarities of smart materials presenting electro- and photo-actuation, advancements of photactuators in microsystem integration are likely to produce synergistic advancements in the integration of electroactuators and vice versa. Ground-breaking OAPAD lay the ground of an incipient field, likely to generate a strong impact in a variety of scientific arenas. Ultimately, we envision optical actuation in multiple environments such as intracellular motors, artificial muscles, and tactile displays for the general public.



Poster Presentations

A study of antimony-doped tin oxide nanofibers

Maritza Reyna & Idalia Ramos
UPR-Humacao

P1

Tin Oxide (SnO_2) is a semiconductor with a large bandgap (3.6 eV) and important properties for electronic and optical applications. The addition of antimony (Sb) can enhance the conductivity of SnO_2. Sb-doped SnO_2 nanofibers have been produced using electrospinning and a solution containing $SnCl_4$, $SbCl_3$ and Cellulose Acetate dissolved in Dimethylacetamide and Acetone. After electrospinning the fibers were sintered in air at 700°C for 2 hours. The fibers morphology and size were analyzed using SEM and showed continuous fibers with diameters ranging from 40 to 1000 nm and lengths of up to several millimeters. The composition and crystallinity of the nanofibers were studied using Energy Dispersive Spectroscopy (EDS) and X-Ray Diffraction. Results demostrate the production of Antinomy-doped Tin Oxide nanofibers. The UV-Vis absorption spectrum was used to calculate a bandgap of approximately 4 eV.

Tin Oxide electrospun nanofibers decorated with silver

Lytzamed Santa[1], Joshua Robles[2] & Idalia Ramos[1]
[1]UPR-Humacao & [2]Petra Mercado High School

P2

The optical and gas sensing properties of metal oxide nanowires can be enhanced with the addition or decoration with metallic nanoparticles. A method described by A. Morril et.al.[Chem Phys Lett, 2009] was used to decorate electrospun tin oxide nanofibers with silver nanoparticles. The fibers were prepared using a precursor solution containing $SnCl_4$ and Cellulose Acetate dissolved in Dimethylacetamide and Acetone. After electrospinning the fibers were sintered in air at 700°C for 2 hours. Before decoration the surfaces of the electrospun tin oxide nanofibers were functionalized growing self-assembled monolayers of 3-aminopropyltriethoxylane (APTES) over them. After the initial treatment the fibers were exposed to colloidal borohydride-reduced silver nanoparticles. The process was implemented using single fibers and mats of nanofibers. Images of tin oxide nanofibers exposed to the colloidal silver nanoparticles for periods of 24, 48 and 72 hours were studied using Scanning Electron Microscopy.

Electrospun zinc oxide nanofibers containing silver particles

P3

Rut Rivera & Nicholas J. Pinto
UPR-Humacao

The goal of this work is to prepare nanofibers of ZnO containing Ag particles. We begin with the precursor solution containing polyvinylpyrrolidone (PVP; Mn 1 300 000; Alfa Co.) as a plasticizer. Our first step was to electrospun the pure PVP sol in water (20wt %) to assure us that nanofibers of this polymer are readily fabricated. In the next step, we dissolved a small quantity of silver nitrate and zinc nitrate in the above PVP sol. This was then electrospun and we obtained nanofibers of PVP containing the silver and zinc precursor. Upon annealing in air at 500C we expect to have zinc oxide nanofibers containing silver particles. The following chemical reactions are expected to take place during the annealing process[1]:

$$2Zn(NO_3)_2 \rightarrow 2ZnO + 4NO_2 \uparrow + O_2 \uparrow \quad (1)$$

$$2AgNO_3 \rightarrow 2Ag + 2NO_2 \uparrow + O_2 \uparrow \quad (2)$$

Once we have prepared the zinc oxide nanofibers containing silver particles we plan to use them to fabricate devices like field effect transistors and Schottky diodes as well as gas and light sensors. The results of this work will be presented in this poster.

[1] D. Lin, H. Wu, X. Qin and W. Pan. *Appl. Phys. Lett.* **95**, 112104 (2009).

Control of diameter and alignment of PLLA/PEG electrospun fibers

Ericka Velez Bonet & Victor Pantojas
UPR-Cayey

P4

Scientists have been extensively studying the use of both synthetic and natural polymer fibers in the preparation of scaffolds for tissue engineering applications. The high surface to volume ratio of fiber meshes enhances the efficiency of mass transport and cell attachment to scaffolds. The making of such fibers is possible by using electrospinning. The structure of these scaffolds is expected to promote cell adhesion, maintain cell functions and organize their growth. Biodegradable polymers such Polyethylene Glycol (PEG) and polylactides (PLLA), are commonly used in biomedical applications. By changing the amount of solvent and the rate of injection for a solution of (80/20) PLLA/PEG, the diameter and morphology of the fibers can be controlled. Also, fiber alignment is desirable in order to control the direction of cell adhesion and growth. The fibers were evaluated by Scanning Electron Microscope (SEM). We show that, by changing the concentration of the solvent in the mixture, we obtained fibers with diameter ranging from 0.2μm to 2μm. By changing the rate of injection where the most viscous solution was injected at a lower rate (0.3mL/hr) and the most diluted solution was higher rate (1.6mL/hr) it was possible to further decrease the range of fiber diameters proving that the diameter of the fibers can be controlled. The fiber alignment was characterized by the order parameter $S = 3\cos^2\theta - 1/2$ where θ is the average deviation from the preferential fiber direction.

Organic-inorganic diodes fabricated using electrospun poly(3-hexylthiophene) fibers and n-doped Si

P5

Stephan Montañez, Rosette González,
Freddy Wong, luis Rosa
& Nicholas Pinto
UPR-Humacao

An organic-inorganic diode was fabricated by using electro spun p-doped poly(3-hexylthiophene)-(P_3HT) fibers and placing one of them on top of a n-doped Si wafer with a thermally grown oxide layer, which had Au electrodes evaporated on its surface. By cleaving the Si wafer on the Au electrodes it leaves an edge with the Au electrodes separated from the Si wafer by the oxide layer. On that edge we place the P_3HT fiber so that it goes over the edge and touches the Si wafer. The p-n junction was formed at the intersection of the P3HT fiber and the n-doped Si. By applying a positive potential to the n-region the p-region lowers the Fermi energy increasing the barrier height , preventing electrons from flowing from the n-doped Si and the contrary happens when the positive potential is applied to the p-region. We tested the diode in air and in vacuum and it operates satisfactorily on both. The P_3HT nanofibers have a high surface area to volume ratio and relatively low turn-on voltage because of that, it makes this device attractive for use as low power consumption diode and gas sensor.

Electrospun nanofibers of poly(vinylidene fluoride-trifluoroethylene)-poly(3,4-ethylenedioxythiophene) composites

Osmarie Martínez, Ariana Bravo & Nicholas Pinto
UPR-Humacao

P6

Nanofibers of PVF_2-TrFE/PEDOT-PSS were fabricated at room temperature using electrospinning, with the thinnest fiber having a diameter of ~15nm. This process for generating PVF_2-TrFE/PEDOT-PSS composite nanofibers is cheap, fast and reliable. The presence of conducting PEDOT-PSS assisted in the fabrication of PVF_2-TrFE nanofibers at low polymer concentrations in DMF and Energy Dispersive X-ray spectroscopy confirmed the presence of PEDOT-PSS in the nanofibers. As a fiber mat, they were electrically conducting and used in the fabrication of a Schottky diode, and the diode parameters were calculated assuming the standard thermionic emission model of a Schottky junction. Being a composite, these nanofibers are promising candidates for use in a variety of applications that can take advantage of the ferroelectric and/or conducting properties of each individual component. In addition, the large aspect ratio and even larger surface to volume ratio of the fibers makes them ideal candidates in the fabrication of miniaturized, low power consumption devices and supersensitive sensors.

Imaging analysis of polystyrene nanosphere masks towards fabrication of nanocapacitors

Melissa D. Santana, Ramon L. Claudio,
Kiazmarie T. Pinto & Josee Vedrine
UPR-Humacao

P7

In this work we explore the use of polystyrene spheres (100 nm) as a single layered mask towards nanocapacitor fabrication. We compare different processing techniques for producing a single layer of spheres that is ordered on silicon substrates. Atomic Force and Scanning Electron Microscopy illustrate spherical arrangement and excellent orientational order on the surface locally, but not globally. Polystyrene masks are then coated with a thin metallic film to produce triangular contacts at the interstices that will ultimately form nanocapacitors.

Electrospun tin oxide nanoribbons crossed with graphene for device and sensor applications

P8

Katherine Carrasquillo[1], Alan.T. Johnson Jr.[2] & Nicholas Pinto[1]
[1]UPR-Humacao & [2]UPENN

Tin oxide nanoribbons having a thickness of ~ 20 nm crossed with graphene have the ability to rectify ac signals. Using a simple electrospinning technique we were able to fabricate in air, tin oxide nanoribbons precursors that were then converted to tin oxide via thermal annealing. These nanoribbons were characterized in a field effect transistor (FET) configuration and were seen to be n-type doped. By simply placing a p-doped graphene layer over the nanoribbbon we were able to fabricate a junction diode. The device was electrically characterized in a FET configuration using a Keithley electrometer and the current- voltage characteristics were non symmetric and resemble that of the diode. Using the back gate bias we were able to tune the diode turn-on voltage by a small amount. This is a very useful feature not common to diodes and expands the possible use of this device to applications other than rectification for examples in sensors. The large surface to volume ratio of the nanoribbons is expected to increase the sensitivity when used as sensors. The simple and cheap method outlined here makes the electrospinning technique very desirable in the fabrication of low power consumption devices and super sensitive gas and light sensors.

Designing a new generation of electrochemical biosensors for the detection of pseudomonas aeruginosa Exotoxin A

Yanira Enríquez & Ana R. Guadalupe
UPR-Río Piedras

P9

Pseudomonas aeruginosa is an opportunistic pathogen and is considered one of the most common bacterium found in nosocomial infections. The capacity of *Pseudomonas aeruginosa* to infect a tissue depends upon the production of virulence factors like enzymes and toxins that damage host cells. One of the virulence factors, in fact the one we are interested in is Exotoxin A. This exotoxin inhibits the protein synthesis in a number of culture cells by catalyzing the transfer of the ADP-ribose of ß-NAD^+ to eukaryotic elongation factor 2 (eEF-2). Apparently this "ADP-ribosylation" of EF-2 inhibits the translocation of ribosomes to mRNA and as a consequence avoids protein synthesis.

We are interested in designing and constructing an electrochemical biosensor for the detection of *Pseudomonas aeruginosa* in hospitals and other settings. A free radical copolymerization of Styrene and NAS (50:50) has been done in THF using AIBN to generate a film on gold and carbon surfaces in order to anchor ß-NAD^+ electroactive analog. The copolymer has been characterized by ^{1}H-NMR, ^{13}C-NMR and FT-IR. The synthesis for the ß-NAD^+ electroactive analog has been done simultaneously using Ferrocene Succinimide. The characterization of the ß-NAD^+ analog has been done using Cyclic Voltammetry, Square Wave Voltammetry, ^{1}H-NMR and ^{13}C-NMR. The voltammograms obtained for the ß-NAD^+ electroactive analog shows two signals, the first one between 300-320mV and the second one in 600mV. The second signal represents the oxidation of the Ferrocene Succinimide which is centered on the ferrocene nucleus while the first band seems to be the oxidation of the Ferrocene in the ß-NAD^+ analog.

Our work is now focused on the full characterization of the ß-NAD^+ electroactive analog and the synthesis of the Styrene and NAS (25:75 and 75:25) copolymer. Our goal is the successful modification of the electrode surface with ß-NAD^+ analog and the electrochemical monitoring of the ADP-ribosylation process mediated by Exo A in vitro.

Electrochemical and spectroscopical characterization of ferrocene chalcones derivatives: cyclic voltammetry, diffusion coefficients, kinetics and UV-visible

P10

Rocío del A. Cardona, Ingrid Montes, Ana R. Guadalupe, Kenneth Hernandez & Myrna R. Otaño
UPR-Rio Piedras

We have synthesized a series of ferrocene chalcones derivatives via Claisen-Schmidt condensation. We are interested in these compounds as electrochemical labels for the development of electrochemical biosensors and as redox mediators for enzymatic reactions. In order to explore the potential bioanalytical applications of these compounds it is important to gain a full understanding of their electrochemical and spectrophotochemical properties.

The electrochemical experiments were done using a three electrodes cell with platinum as working electrode, Ag/AgCl (3 M NaCl) and nichrome as reference and auxiliary electrodes respectively. The experiments were done in TBAP (0.1 M)/acetonitrile under a nitrogen atmosphere. The data showed that all compounds exhibit a quasi-reversible electrochemical behavior and reversible chemical behavior as evidenced by ΔEp and Ipa/Ipc values. The formal potential for these compounds range between (665-774) mV which are (200-300) mV higher than Ferrocene formal redox potential. The electron transfer rate were calculated by using the Nicholson method and are at (2.0-4.4) x 10^{-2} cm/s, which is comparable with values reported on the literature for Ferrocene under similar experimental conditions. The diffusion coefficients for all compounds are on the order of (1.65-3.7) x 10^{-5} cm^2/s and the number of electrons transfer per mole is equal to one. The UV-Vis spectra showed characteristic bands for aromatic systems in the UV region (200 and 280) nm and bands in the visible (400 and 500) nm which are in accordance with p-extended systems. The calculated molar absorbance coefficient values range (2.1-7.5) x 10^4 L/(mol.cm) for the ultra-violet bands and (1.8-17.6) x 10^2 L/(mol.cm) for the visible bands.

Our future work consists in using the most promising compounds as electroactive label to detect DNA hybridization and as redox mediators for compounds of biological interest

Development of a nucleic acid biosensor for the electrochemical detection of salmonella

Madeline Díaz[1], Arelys Rosado[1], Joselyn del Pilar[1], Esther Z. Vega[2] & Ana R. Guadalupe[1]
[1]UPR-Río Piedras , [2]UPR-Humacao

P11

Waterborne and foodborne diseases are one of the principal public health problems worldwide. Our particular interest is the development of nucleic acid biosensors (NAB) for the detection of pathogenic microorganisms in food and water samples. In this research, we report on the development of a NAB prototype using a polymer modified electrode surface together with an electroactive ferrocene (Fc) derivative (Scheme 1). To test this prototype, we are using a 35 mer sequence of the OmpC gene from Salmonella as our probes. This oligo has been modified to anchor it in a polystyrene-modified carbon surface as an electrode.

We have synthesized several PS films and anchor nucleic acid sequences with different lengths at gold and carbon surfaces. Non contact mode AFM and XPS were used to monitor each step of the NAB preparation, from polymer modification to oligos hybridization. After modification, the AFM images showed a surface completely coverage by the polymers with a smooth morphology. The images also showed the existence of globular morphology in the ODN film and partially porous film after hybridization. The XPS analysis confirmed the morphological changes observed in the AFM images after the hybridization, which results in the partial exposure of the gold surface. The hybridization event has been detected electrochemically by the conventional method, which is modifying the target with Fc-NHS. We observed a small current at the potential for the Fc oxidation without signal amplification. We study the variations on ionic strength with respect to sensitive hybridization detection.

We expect to produce a methodology for the construction of electrochemical biosensors based on the use of *Salmonella* DNA-functionalized polymeric films with spatial resolution, high reproducibility and high sensitivity. Our experiments are now centered on testing the label-free hybridization design and the synthesis of bimetallic label complexes.

Electrospun polymer nanofibers containing antibiotics

P12

Yelitzzah M. Fernández[1], Yarely C. Dávila[1] & Nicholas J. Pinto[2]
[1]Bellas Artes high School & [2]UPR-Humacao

Electrospinning is a method used for the production of fibers. In this method, a high voltage is used to create an electromagnetic field between a polymer solution and a collector plate. A high voltage applied to the anode will be in contact with the polymer solution placed in a hypodermic needle, and the collector plate will be grounded. When the voltage is increased, the electromagnetic field between the needle tip and the cathode will increase simultaneously provoking a force that will push the polymer solution toward the cathode. With the help of a syringe pump that will push the piston slowly, a drop of the solution will fall off the needle tip every five or ten seconds, this electromagnetic force will overcome the surface tension of the drop resulting in a fine jet emanating from the needle. Meanwhile, the solvent will evaporate and the polymer fibers will be adhered to the cathode situated few centimeters from the needle. We have used this method to create polymer nanofibers adding antibiotics with the purpose of accelerating the natural healing process when used to cover wounds. One of the advantages that nanofibers have over thin films is the enhanced surface to volume ratio. The electrospinning technique is perfectly suited for the fabrication of non woven fibers mats that could be used to cover open wounds (artificial skin). With this in mind, we have tried to incorporate antibiotics into the electrospun polymer fibers. The central idea being that an open wound would tend to heal faster if covered with such a medicated porous wrap. We believe that the large surface area will lead to more efficient use of the antibiotics as the porosity of the fibers will simultaneously allow for liquid evaporation and formation of the healing scab over the wound. We have successfully used polyethylene oxide as the base polymer that is non-toxic and incorporated the common antibiotic Neomycin into the fibers using electrospinning. The results of this research will be presented in this poster.

Preparation and characterization of Mn0.8Zn0.2Fe2O4/polyaniline EB nanocomposites for EMI shielding applications

María A. Abreu-Sepúlveda[1], Boris Renteria-Beleño[2], David Mazuera[2] & Oscar Perales[2]
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P13

Several methods have been developed in order to avoid the electromagnetic interference (noise) caused by popular circuits as computers and cell phones, among others. The objective of this research was to prepare and characterize a material which shielding behavior protects the equipment of EMI disturbance. The active materials, Polyaniline Emeraldine Base (Pani EB) and Mn0.8Zn0.2Fe2O4 were characterized separately using different techniques as Thermogravimetric Analysis, Vibrating Sample Magnetometer and X-Ray Diffraction. The surfactant Dodecyl Benzene Sulphonic Acid (DBSA) was mixed with the ferrite particles to protect them of the HCl involved in the synthesis process of the Pani. The TGA study showed the decomposition temperature of each material and compound was between 200°C to 400°C, the magnetization of the Mn-Zn ferrite was found to be 54.2emu/g, while the composites of Pani-ferrite filtered with ethanol and HCl had 0.2emu/g and 0.011emu/g, respectively. The DBSA protected the ferrite particles during the synthesis process, but the magnetization after the filtration with HCl was almost zero. Finally, films of Pani in N-Methyl 2-Pyrrolidone (NMP) were prepared using slow solvent evaporation in a hot plate at 60 °C, those films were tested using Dynamical Mechanical Analysis (DMA).

Computational & graphical representation of electrostatic potentials using VMD & GPU

P14

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This work presents results of the use of a Graphical Processing Unit (GPU) to calculate and represent the electrostatic potential and atoms charges in a molecular dynamics simulation. A previously created tool with a graphical user interface (GUI) for the Visual Molecular Dynamics (VMD) calculates the atoms charges by dividing the system in a user defined grid and calculating an using sums of charges in each box of the grid as a base for the computation. The GUI makes a representation of the atoms charges using a false color scale. The user can also select the residues that are used in the representation.

The extension shows the electrostatic potentials using the VMD 3D display, using another false color scale. This part consumes a large amount of CPU time. As part of the upgrade, we created new methods for accelerating the time spent in data processing. The original version used a sequential code in C++. This computational complexity of the evaluation of the electrostatic potentials is O(N3). As part of the upgrade, we developed a new code written in CUDA to use NVIDA GPUs. Initial tests using a NVIDA Tesla GPU with 512 processing units showed an improvement in speed by a factor of 8.

Then the data movement between Python and CUDA was improved. We created a method of passing the data using sockets instead of files. This reduces, in cases where a simulation contains a large numbers of atoms, the risk of producing huge files, and improves the performance.

Finite element method simulations of composite materials

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P15

A *composite* material consists of a mixture of a base material called the *matrix*, with grains of other materials called the *inclusions*. These materials are very common in engineering applications like the construction industry. Composite materials have also been used for the production of capacitors with different type of military applications, yet the role of the composite in the efficiency of such a device is not well understood. Modeling composite materials is difficult due to the random nature of such mixtures. However if some controls are established during the production process, it is reasonable to assume homogeneity and isotropy. Models for composite materials have been proposed in the literature, for example by Hill (1972), and can be either random or periodic. The main goal of the present work is to study numerical methods based on the finite element method to determine the mechanical properties of periodic composite materials. At the moment we have been studying a simplified version of this problem for a nonlinear Poisson type equation. Since the constitutive function for a composite material is a piecewise defined function of the constitutive functions of the matrix and inclusions, we take the coefficients in our Poisson type equation to be nonlinear piecewise defined functions, changing behavior in the regions simulating the matrix and inclusions. We present some simulations for this simplified problem that resemble materials with voids (empty inclusions) and with (filled) inclusions.

Operations to Generate Adyacencies of State Transition Digraphs Associated to Polymers Modeled by Self Avoiding Paths and Polygons

P16

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Self-avoiding walks (SAW) and polygons (SAP) defined over regular grids have been used to model polymers since early last century. A common method for studying statistical properties of SAWs and SAPs drawn over rectangular strips consists of constructing diagrams called column states to describe changes in the paths between columns of points. We approach the study by associating a digraph grids of specified width by taking the set of column states as its vertex set and directed edges defined according to allowable column states successors. Previous results include a set of theorems that establish necessary and sufficient conditions for determining whether pair of vertexes in SAPs digraphs are adjacent or not. In this work the result of a search of adjacencies that are not described by those criteria, a necessary step toward establishing new criteria for adjacencies is presented . In a similar tone, a set of five new theorems that describe adjacencies on SAW digraphs based on the adjacencies found in SAPs digraphs are presented. Finally examples of adjacencies that are not described by those criteria are presented.

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