MRS FALL MEETING

November 25-30, 2018

Boston, MA

SESSION BI01.06: Poster Session: Sustainable Development in Materials Science and Related Societal Aspects

BI01.06.05

Investigating the Effects of Different Spun-Cast and Molded Polylactic Acid (PLA) and Polystyrene (PS) Composites on the Proliferation, Differentiation and Biomineralization of Dental Pulp Stem Cells Kuan-Che Feng¹, Ethan Ho², Bhuvna Murthy³, Rushi Patel⁴, Antony Deluxe⁸, Wenqi Zhao⁵, Benjamin Chang⁶, Nicholas Zumba⁷, Chung-Chueh Chang¹, Marcia Simon¹ and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Northfield Mount Hermon School, Gill, Massachusetts, United States; ³Huron High School, Ann Arbor, Michigan, United States; ⁴Herricks High School, New Hyde Park, New York, United States; ⁵Milton Academy, Milton, New York, United States; ⁶Woodbridge High School, Irvine, New York, United States; ⁷Columbia University, New York City, New York, United States; ⁸Wheatley High School, Old Westburry, New York, United States.

Polymers are known to be more combustible than other structural materials, and hence flame retardant formulations are frequently added. Recently it has been shown that many of these formulations, especially those containing halogenated compounds, are toxic and leach into surrounding water and soil. This concern is even more pressing when biodegradable polymers are used, where the degradation process facilitates the environmental release of the toxins.

Here we report on a study of the toxicity of resorcinol diphosphate, RDP, a phosphorous based flame retardant additive. RDP is easily compounded into homopolymers or polymer blends when adsorbed onto clay, where it also facilitates compatibilization.

In this study, we show that when included into PLA, RDP appears to have no deleterious effects on cell adhesion, proliferation, and differentiation. When RDP-Clay is added to polystyrene, it has an advantageous influence. Cells do not adhere to PS, but when RDP Clay is added, cell plating efficiency and cell proliferation is drastically improved and the doubling time is comparable to that of the cells plated on PS. In contrast to the cells on PS, those on the PS-RDP-Clay and PLA-RDP-Clay scaffolds underwent differentiation, where large amounts of hydroxyapatite deposits were found. With the appearance of what is believed to be hydroxyapatite deposits (biomineralization), RAMAN spectroscopy will be used to determine any possible developments of an extracellular matrix on the PS-RDP-Clay and PLA-RDP-Clay scaffolds. Additionally, RT-PCR will be conducted on days 28 and 42 in order to evaluate the presence of all genes that may be associated with osteogenic or odontogenic differentiation. Even though further in-vivo testing is required, these results indicate that the probable toxicity of RDP is low, since RDP-Clay preserves both cellular proliferation and function.

TP02.03.15

3D Printed Polypropylene Nanocomposites for Thermal and Electrical Conductivity Applications <u>Yuval Shmueli</u>¹, Vedant Singh², Daniel Chao³, Ahmed Shata¹, Mustafa Zaidi¹ and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²The Wheatley School, Westbury, New York, United States; ³Hunter College High School, New York, New York, United States.

Polypropylene (PP) is a common polymer being used in many products in all industrial fields. However, due to its relatively high crystallinity percentages it has difficulties in being produced in the emarging plastics production technology -3D printing. In this work we show how crystallinity in the printed structure can be advantage due to its orientation that has great potential for conductance applications and also can increase the mechanical properties. We also show how incorporation of thermal conductive nano-fillers as Graphene nano platelets (GNPs) and hexagonal Boron Nitride (hBN) at 0, 5 and 10 wt% combined with the polymer orientation can lead to optimal thermal and electrical conductivity properties of the printed products. We modified the Gcode input to the printer and studied the printing process in order to study the printing conditions for optimal interfilaments fusion and printed product properties.

We used high resolution infra-red thermal camera to measure the thermal conductivity of the printed structure. We also used high voltage resistivity meter to measure the electrical properties. In addition, we used small angle X-ray scattering (SAXS) microbeam to study the macrostructure in the printed structure as function of the radial position from the filaments "skin" and interface to the "core" of the filaments. Our results show the significant improvement to the conductivity properties when the nano-fillers are being introduced to the matrix and in particular, the graphene nano platelets.

We Acknowledge support from the National Science Foundation (Inspire Award No. 1344267) and The Morin Foundation Trust.

10:45 AM BI01.08.02

A Novel Fire Retardant Solution to Mitigate the Onset of Wildfires <u>Yuan Xue</u>¹, Xianghao Zuo¹, Joshua Vilkas², Pik Hoi Lam³, Nicole Jacobsen⁴ and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Hebrew Academy of Nassau County High School, Uniondale, New York, United States; ³Wilson Area High School, Easton, Pennsylvania, United States; ⁴Plainedge High School, Massapequa, New York, United States.

The dangers of wildfires are brought to attention as they frequently ravage wooded areas like California and Greece. The current resolution is reactive rather than preventive, and involves dropping chemicals after the start and expansion of the fire. Additional concerns include the application of non-eco- friendly ingredients to quench the fires. The goal of this research is to engineer aqueous solutions that are sprayed onto leaves prior to the onset of fires to inhibit fires from spreading uncontrollably. Here we describe the results of a formulation that was used on the leaf species, *Cornus kousa*, a subspecies of the *Cornus*, or Dogwood family.

The experiments were conducted on three categories: fresh picked leaves, oven-dried leaves, and naturally fallen leaves. FTIR analysis of the leaves indicated that fresh leaves consisted of water (2/3 of the mass) while the dried leaves were predominantly of cellulose. Fresh leaves were coated with a thick waxy layer, while the drying process removed some of the surface wax. Different solutions were first formulated where contact angle goniometry was used to optimize the wetting properties for both dry and fresh leaves and viscometer was used to determine the optimal viscosity for spray applications.

The solutions were then applied by spraying onto fresh leaves and piles of dried leaves. Burning tests were performed both on leaf piles, and individual leaves, using a propane torch. The flame was applied continuously for five seconds and then removed, and the time to self-extinguish was recorded together with the extend of the spread of the fire.

Results indicated that for fresh leaves, in the absence of the spray, the fire persisted till at least ³/₄ of the mass was consumed and for the dried leaves the entire mass was consumed before the fire was removed. With the addition of the spray, the fire self-extinguished immediately after the flame was removed, and the fire during the application of the flame consumed less than 25% of the mass. Similar results were obtained for both wet and dry leaves. FTIR and RAMAN spectroscopy was performed at each stage in the testing in order to determine the underlying mechanism leading to the flame retardant properties.

The toxicology of the solution and the individual components is being tested on grass and vegetable plants. Preliminary data, thus far, had not found any significant differences in root size or germination rate between the control plants culture and those watered with the undiluted solutions. The results of ongoing experiments regarding sequestration of the chemicals in the leaves and fruits will be presented.

SESSION BM01.03: Poster Session: 3D Printing of Passive and Active Medical Devices

BM01.03.12

Study of Fusion in 3D Printing of PLA/Graphene Composites <u>Yuval Shmueli</u>¹, Xiaoxin Wang², Steven Wu³, Derek Zheng⁴, Lan Jiang⁵, Caroline Zeng⁶, Dilip Gersappe¹, Miriam Rafailovich¹, Matthew York⁷ and Zhuolin Xia¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Padua Franciscan High School, Parma, Ohio, United States; ³Clear Lake High School, Houston, Texas, United States; ⁴Monta Vista High School, Cupertino, California, United States; ⁵University High School, Irvine, California, United States; ⁶Wayzata High School, Plymouth, Minnesota, United States; ⁷Case Western Reserve University, Cleveland, Ohio, United States.

Fused deposition modeling (FDM) printing is an emerging 3D printing technology in which thermoplastic filaments are extruded and deposited in certain manner according to computer input design. Polylactic acid (PLA) is a common biodegradable polymer being used in FDM printing and has great potential to be the main component in future biomedical devices. However, since it has poor thermal conductivity properties it is often leads to failing interfilaments fusion and hence reduces the overall product mechanical and functional properties.

In this work we incorporate graphene nano platelets (GNPs) to examine their effect on the thermal profiles during printing and the resulted mechanical properties. We studied the conditions of different nozzle temperatures and varied the distance between adjacent filaments and between deposited layers by adjusting the Gcode input to the printer. We used high resolution infra-red thermal camera to monitor the temperatures at the printing process. Then we correlated these profiles with (scanning electron microscopy) SEM analysis and dynamic mechanical analysis (DMA) properties of the printed structure. We also used microbeam small angle X-ray scattering (SAXS) measurements to study the macrostructure of the printed filaments as function of the radial position from the interfilaments interface to the filaments core. In addition, we modeled the temperature profiles and the flow mechanics of GNPs flow in the polymer matrix using Lattice Boltzmann Modeling (LBM).

We show the great effect of GNPs inclusion on the fusion process while printing and how it affects the resulted properties and can be used in future potential applications. The experimental results combined with the modeling results enable us to present the optimal conditions and composition to improve the fusion and hence the strength of the printed structures.

We Acknowledge support from the National Science Foundation (Inspire Award No. 1344267) and The Morin Foundation Trust.

BM01.03.14

The Effect of Surface Roughness of 3D-Printed PLA Scaffolds on the Cell Attachment, Proliferation and Differentiation of Dental Pulp Stem Cells Kuan-Che Feng¹, <u>Wenqi Zhao</u>², Benjamin Chang⁴, Bhuvna Murthy⁷, Ethan Ho⁵, Rushi Patel³, Antony Deluxe⁶, Marcia Simon¹ and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Milton Academy, Milton, Massachusetts, United States; ³Herricks High School, New Hyde Park, New York, United States; ⁴Woodbridge High School, Irvine, California, United States; ⁵Northfield Mount Hermon School, Gill,Massachusetts, United States; ⁶Wheatley High School, Old Westbury, New York, United States; ⁷Huron High School, Ann Arbor, Michigan, United States. Three-dimensional (3D) printed scaffolds provide a promising approach in the field of tissueengineering for its ability to precisely control scaffold architecture at the micron-scale. Previous studies have shown that topographical features on the surface of scaffolds can determine the efficiency of cell attachment and proliferation; yet, little is known about their effect on cellular differentiation. Here, we aimed at investigating the influence of the surface roughness of 3Dprinted polylactic acid (PLA) scaffolds on cellular response.

Sub-micron scale roughness on 3D FDM printed structures can result from "shark skin" formation, which were shown to be a result of slip-stick instabilities during fiber extrusion when attractive forces were present between the polymer and the extrusion nozzle. Here we first present a quantitative analysis of shark skin formation in PLA filaments as a function of the printing speed and nozzle temperature, where the roughness was characterized using atomic force microscopy. We then plated dental pulp stem cells on scaffolds printed at different speeds and with different roughness amplitude. Control samples were produced by molding PLA between Kapton sheets, minimizing the surface roughness. In all cases the extend of biomineralization in the absence of dexamethasone, was higher on the printed substrates, than equivalent PLA substrates produced via molding. qRT-PCR of marker genes (ALP, OCN, DSPP) demonstrated significant differences in the cell response and differentiation lineage between molded and printed substrates. Differences were also observed between samples with different sharkskin amplitude and underscoring the influence of surface morphology on differentiation outcome. These results illustrate the the challenges in production of reproducible materials for tissue culture when 3D printing technologies are employed.

BM01.03.15

Study of Hexagonal Boron Nitride (hBN) in Fused Deposition Modelling (FDM) 3D Printing <u>Won II Lee</u>¹, Yuval Shmueli², Young-Soo Seo¹ and Miriam Rafailovich²; ¹Nanotechnology and Advanced Materials Engineering, Sejong University, Seoul, Korea (the Republic of); ²Materials science and chemical engineering, Stony Brook University, The State University of New York, Stony Brook, New York, United States.

Hexagonal boron nitride (hBN) is two dimensional ceramic material with excellent chemical, physical and mechanical properties. Although it is an electrical insulator, it has high thermal conductivity, thermal stability and also it is not toxic and biocompatible. Therefore, this innovative material has the potential of being used in variety of applications.

We incorporated hBN in a polylactic acid (PLA) and polypropylene (PP) matrix in 5 and 10 wt% to study the effect in the 3D printing process and for potential thermal management applications. Dynamic mechanical analysis measurements showed improvement in the mechanical properties and enhance ductility of the printed structure. The presence of the nanoparticles leads to better printing resolution and filaments fusion due to the confinement in the extrusion in the printing process. The hBN did not prevent and interfere with the polymer chains diffusion and affect the filaments fusion process. We measured thermal conductivity properties using infrared thermal camera and compared different printing orientations and molded samples. We saw that addition of hBN improve the thermal conductivity by approximately 10 % comparing to the pure polymer and that the heat conductance is enhanced with the filament orientation relatively to the molded structure with no orientation. We conducted in-situ WAXS measurements simultaneously with high resolution infrared thermal imaging to study the crystallization forming in the matrix. The results showed that addition of hBN did not cause and effect in the crystalline formation comparing to the pure polymer. In the future we will introduce boron nitride nanotubes (BNNTs) into the polymeric matrix to examine their effect on the printed matrix. We will also perform chemical surface modification of both types of the nanoparticles to examine if it will improve the compatibility between the particles and the polymer matrix and by that improving even more the

mechanical and conductance properties.

BM01.03.16

Characterization of Antibiofilm Activity of Silver Nanoparticles Synthesized *In Situ* **on 3D Printed Polylactic Acid Scaffolds** Michael Cuiffo¹, Stephen Walker¹, Yuval Shmueli¹, Fan Yang¹, <u>Anastasia Popova²</u>, Isha Brahmbhatt³, Kuan-Che Feng¹, Adriana Pinkas-Sarafova¹ and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Hackley School, Terrytown, New York, United States; ³Ardsley High School, Ardsley, New York, United States.

Biofilms are bacterial communities highly resistant to antibiotics, biocidal agents, and human immune system. Microorganisms that grow on medical devices form biofilms, and once formed they cannot be completely removed. The need for prevention of biofilm formation and growth leads to different approaches for the modification of materials used for medical devices. Silver nanoparticles, with known antimicrobial properties, have been used to modify polymers. Since silver nanoparticles express their antimicrobial properties by releasing silver ions, when mixed with a polymer before device preparation, the ion release level will be limited by the degradation of the polymer. Polylactic acid (PLA) is a biodegradable and FDA-approved polymer for use in numerous resorbable surgical devices. The Brunst method has recently been patented as an accessible and inexpensive method for in situ synthesis of silver nanoparticles as a coating on PLA. This coating can promote a rapid and prolonged release of silver ions able to inhibit biofilm formation. PLA scaffolds were printed using two 3D printers, a Makerbot Replicator 2X and Ultimaker 2 Extended+, with corresponding filaments, and characterized with a laser microscope and FTIR. The Brunst method was used with two concentrations of AgNO3 (0.1M and 0.01M) and 0.001M NaBH4 for the in situ deposition of silver nanoparticles. We tested the ability of the PLA-AgNO3 scaffolds to inhibit biofilm formation and growth against two strains of bacteria, Staphylococcus aureus (gram-positive) and Escherichia coli (gram-negative). The PLA-AgNO3 scaffolds were also evaluated for the interaction of the modified surfaces with Dental Pulp Stem cells (DPSCs).

We found significant differences in surface chemistry and roughness of scaffolds produced by different printers. PLA scaffolds coated with 0.1 M nanoparticle showed significantly smaller size of the biofilms for both microorganisms than the one with 0.01 M nanoparticles. Bacterial adhesion and biofilm formation was higher on Ultimaker 2 Extended+ printed scaffolds for both strains. The DPSCs had a similar correlation and attached better to the Ultimaker samples in comparison to the Makerbot samples.

SESSION BM01.05: 3D Printing of Passive and Active Medical Devices IV

1:30 PM BM01.05.01

In Situ **X-Ray and Thermal Characterization of FDM 3D Printing** <u>Yuval Shmueli</u>³, Jiaolong Jiang³, Thomas Howell³, Ellen Wachtel¹, Gad Marom², Dilip Gersappe³ and Miriam Rafailovich³; ¹Weizmann Institute of Science, Rehovot, Israel; ²The Hebrew University of Jerusalem, Jerusalem,

Israel; ³Stony Brook University, The State University of New York, Stony Brook, New York, United States.

Fused deposition modeling (FDM) printing is an emerging 3D printing technology in which thermoplastic filaments are extruded and deposited in certain manner according to computer input design. FDM is a rapidly developing new area where new methodology is required to explore phenomena far from equilibrium. In this study, we use *in-situ* synchrotron X-ray scattering and high resolution infra-red imaging to study in-situ the relationship between the extrusion parameters, the filaments deposition directionality and the internal structure of the nanocomposite. In two steps study we place first "home-made" extrusion setup and then open-walls 3D printer in

the beamline.

The results are then compared with Lattice Boltzmann Modeling which simulates the welding between filaments as a function of nozzle parameters, printing protocols, and the system thermodynamical response function. In filled systems, using in-situ X-rays scattering, we observed the effect of extrusion shear forces on the orientation of the nanoparticles and the influence of the particle/polymer interactions on the polymer crystallization. This phenomenon ("Transcrystallization") leads to templating of the polymer crystalline structures by the fillers which, we show, can enhance the thermal, mechanical and electrical properties of the printed nanocomposite structures, under directional control by the printing algorithm. The results of insitu printing measurements show how the parameters of sample temperature, printing orientation and materials composition affect the internal structure and crystalline structure formation.

We Acknowledge support from the National Science Foundation (Inspire Award No. 1344267) and The Morin Foundation Trust.

SESSION BM04.06: Poster Session II: Biomaterials for Regenerative Engineering

BM04.06.17

Engineering Titanium Substrate by Atomic Layer Deposition for Dental Pulp Stem Cells Proliferation and Differentiation Studies <u>Ya-Chen Chuang</u>¹, ², Likun Wang¹, Marcia Simon³ and Miriam Rafailovich¹; ¹Materials Science & Engineering, Stony Brook University, The State University of New York, Stony Brook, New York, United States; ²ThINC Facility, Advanced Energy Center, Stony Brook, New York, United States; ³Oral Biology & Pathology, Stony Brook University, The State University of New York, Stony Brook, New York, United States.

Stem cells are sensitive to both chemical and mechanical changes in the environment, which proliferation and differentiation depend on three main factors: the type of stem cell, the underlying scaffold, and the signaling molecules added. It has been shown that stem cells isolated from the dental pulp (dental pulp stem cells (DPSCs)) can differentiate and express markers of odontoblasts, osteoblasts, adipocytes or neuronal cells when they are grown in specific inducing media. However, the external chemical inducers such as steroids can cause adverse side effects such as hyperglycemia and a weakened immune system in clinical studies. Therefore, we focus on engineering the underlying substrates to induce DPSCs differentiate along the desired pathway without external chemical inducers added. Titanium, a material used as dental implant, has shown to promote its osseointegration with specific surface treatment to manipulate its surface roughness and topography. Herein, we introduce a new method to fabricate titanium substrate by atomic layer deposition (ALD), which deposits a homogeneous 2~3nm thickness of titanium on silicon wafer substrates. Due to surface chemistry changed, DPSCs have shown to proliferate well on ALD titanium substrates compared to bare silicon surface. At week 4, biomineralization were characterized by SEM/EDS and Raman spectroscopy. RT-PCR was also used to identify odontogenic and osteogenic differentiation markers. The results showed that biomineralized deposits (Ca/P) along with collagen fibers were observed on ALD titanium substrates, and RT-PCR results showed that osteocalcin (OCN) was upregulated from week 2 to week 4 but Dentin Sialophosphoprotein (DSPP) expression remained low over 4 weeks. It suggests that DPSCs growing on ALD titanium surface might induce them to differentiate along osteogenic pathway. The ALD method provides a fast and easy process to coat a homogeneous thin layer of titanium on the substrate, where only surface chemistry changes but which roughness and topography remain the same. This method could be a potential application to coat a thin layer on titanium on any biomaterial to further promote stem cells differentiation and proliferation.

[We would like to thank the NSF-INSPIRE program (Grant #1344267).]

BM04.06.18

Substrate Mechanics in Combination with Nanoparticles Effects on Dental Pulp Stem Cells Proliferation and Differentiation Ya-Chen Chuang¹, ², Chung-Chueh Chang², Marcia Simon³, Miriam Rafailovich¹, Samantha Ying⁴ and <u>Mindy Li⁵</u>; ¹Materials Science and Engineering, Stony Brook University, Stony Brook, New York, United States; ²ThINC Facility, Advanced Energy Center, Stony Brook, New York, United States; ³Oral Biology & Pathology, Stony Brook University, The State University of New York, Stony Brook, New York, United States; ⁴South Side High School, Hempstead, New York, United States; ⁵Princeton High School, Princeton, New Jersey, United States.

Stem cells are sensitive to both chemical and mechanical changes in the environment, which proliferation and differentiation depend on three main factors: the type of stem cell, the underlying scaffold, and the signaling molecules added. It has been shown that stem cells isolated from the dental pulp (dental pulp stem cells (DPSCs)) can differentiate and express markers of odontoblasts, osteoblasts, adipocytes or neuronal cells when they are grown in specific inducing media. In our previous study, we have shown that monodisperse polybutadiene (PB) can be used to produce biocompatible flat thin films with different surface mechanics by simply altering the film thicknesses where surface chemistry remains the same. We have also shown that DPSCs can sense and adjust their cell mechanics accordingly to the underlying substrate mechanics. In addition, without the addition of inducing media, dexamethasone, biomineralized deposits and upregulation of osteocalcin (OCN) gene marker were observed on hard PB surfaces. In contrast, extremely low level of biomineralized deposits and OCN were observed on the softer PB surfaces. On the other hand, the rise of nanotechnology also promotes the study on the effects of nanoparticles (NPs) on stem cell and shows that nanoparticles can also offer a means of regulating cell function. However, stem cells are extremely sensitive to the extracellular signals where the stimuli from substrate mechanics and NPs should be studied simultaneously. Hence, in this study, we want to investigate how DPSCs proliferate and differentiate when both substrates mechanics and NPs cues were involved. Briefly, TiO2 NPs (0.1 mg/mL) were added post-plating onto soft and hard PB substrates after DPSCs fully attached. Cell proliferation and cell mechanics were measured at week 1 by hemocytometer and shear modulation force microscopy (SMFM). At week 4, biomineralized deposits were characterized by SEM/EDS and Raman spectroscopy. RT-PCR was also used to identify odontogenic and osteogenic differentiation markers. The results showed that with TiO₂ NPs added, collagen fibers along with biomineralization were deposited on the substrates, and it showed up-regulation of OCN gene at the later stage of differentiation process no matter the substrate is soft or hard. The results suggest that TiO₂ NPs overwrite substrate mechanics effect and dominate DPSCs differentiation in this system, which could be a potential application for nanoparticles using as stem cell differentiation inducer.

[We would like to thank the NSF-INSPIRE program (Grant #1344267).]

SESSION BM04.07: Polymeric Biomaterials for Regenerative Engineering II

8:30 AM BM04.07.02

Investigating the Effects of Substrate Mechanical Patterns on Proliferation and Differentiation of Dental Pulp Stem Cells <u>Ya-Chen Chuang</u>⁴, 1, Chung-Chueh Chang¹, Jessica Hofflich⁴, Grace Liu², Albert Zhu³, Marcia Simon⁵ and Miriam Rafailovich⁴; ¹ThINC Facility, Stony Brook University, Stony Brook, New York, United States; ²Bayview Secondary School, Richmond Hill, Ontario, Canada; ³Our Lady of

Lourdes High School, Poughkeepsie, New York, United States; ⁴Materials Science and Engineering, Stony Brook University, Stony Brook, New York, United States; ⁵Oral Biology and Pathology, Stony Brook University, Stony Brook, New York, United States.

Stem cells isolated from the dental pulp (dental pulp stem cells (DPSCs)) were shown to differentiate and express markers of odontoblasts, osteoblasts, adipocytes or neuronal cells when they sense the environmental changes such as the underlying scaffold and the signaling molecules added. In our previous

study, we have shown that monodispersed polybutadiene forms a convenient biocompatible scaffold, to which the cells can adhere without additional coatings. Furthermore, we showed that the substrate modulus obeyed a continuously differential function where the film modulus could be varied by more than an order of magnitude simply by changing the film thickness. DPSC plated on these PB substrates were able to adjust their moduli in response to the film thickness, obeying the same functional form as the PB films. Yet, despite the continual change in cell hardness, an abrupt change occurred for substrates moduli greater than 2.3 MPa when large amounts of biomineralized deposits were observed after 28 days.

RT-PCR analysis indicated that the substrate mechanics induced differentiation of the cells without any additional chemical inducers. Florescent immunohistochemically staining indicated that all the cells in the tissue that formed expressed OCN, a protein necessary for biomineralization and an indicator for osteogenic differentiation, on thin, hard PB films, while no OCN was found in cells on the softer, thick PB films. Hence direct contact with the hard substrate was only required for one of the layers, and the effect was propagated further into the films.

Scaffolds with mechanical patterns surface patterns were then produced with length scales ranging from the macro to the nanoscale. The patterns were produced simply by imprinting in the Si wafer and adjusting the film thickness, without chemical cross linkers introduced into the PB films. Hence the influence of purely mechanical heterogeneity could be probed. In the case of microscale patterns, the results indicate that the influence of the substrate mechanics is communicated within the tissue via cell-cell contact. In the case where both hard and soft patterns were present, in a manner with enabled cell-cell contacts to form between patterns, no biomineralization was observed. If cell-cell contacts were prevented, differentiated and non-differentiated cells were able to coexist within a single culture, where the phenotype was governed by the substrate mechanics. This study is important when applying printed scaffolds as dentin/tooth regenerative biomaterials, which surface is rough and the mechanics is not homogeneous.

9:00 AM BM04.07.04

Enhancing Oseointegration on Biodegradable Polymer Scaffolds with ALD Deposition of Titania <u>Kuan-Che Feng</u>¹, Adriana Pinkas-Sarafova¹, Likun Wang¹, Ya-Chen Chuang¹, Linxi Zhang¹, Chung-Chueh Chang², ¹, Marcia Simon¹ and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Advanced Energy Center, ThINC Facility, Stony Brook, New York, United States.

Fused deposition modeling (FDM) is a rapidly growing method for device fabrication. The technique is inexpensive and the product, such as bone inserts, dental devices, can be printed directly from CT scans or impressions, and hence specifically tailored for the individual. However, from the former study shows that the cell did not attach well on the FDM printed surface due to the roughness of FDM printed surface and hydrophobicity of the polylactic acid (PLA). In this study we produced FDM printed scaffolds that were then coated with titanium dioxide via the atomic layer deposition (ALD) method. TiO₂has been shown in numerous studies to enhance osseointegration. Hence by this technique one can produce scaffolds that are at once biodegradable,

and yet support osteogenic or odontogenic differentiation. In order to probe this concept, we plated dental pulp stem cells on these scaffolds, incubated for 28 days, in media with glycerol phosphate, but without the commonly used induction factor, dexamethasone. The culture was then harvested for qRT-PCR and the surfaces were imaged with scanning electron microscopy. Cell mobility, proliferation, and differentiation were studied and significant differences in both biomineralization and differentiation were observed between coated and uncoated surfaces.

11:30 AM BM04.07.12

Analyzing the *In Vitro* Viability of Novel Gelatin-Pluronic® F127 Hybrid Hydrogels as Cell Barrier Membranes for Guided Bone Regeneration Following Periodontitis Juyi Li², <u>Kevin</u> <u>Chen</u>¹, Joon Young Lee³, Aaron Sun⁴ and Miriam Rafailovich²; ¹Mira Costa High School, Manhattan Beach, California, United States; ²Stony Brook University, Stony Brook, New York, United States; ³Seoul International School, Seongnam City, Korea (the Republic of); ⁴Ed. W Clark High School, Las Vegas, Nevada, United States.

Periodontitis, or conventionally "Gum Disease," begins with the infection, and subsequent inflammation, of gingival tissue and is currently the leading cause of tooth loss in the United States. Though there exists a wide array of methods for treatment of periodontitis, one of the most effective is guided bone regeneration (GBR). GBR consists of applying a barrier membrane to separate inflamed gingival tissue from bone, restricting invasion and allowing regeneration of osteoblasts. Current barrier membranes, however, do not fulfill all the desired properties of high biocompatibility, cell impermeability, and, in particular, high mechanical strength. As such, the following study synthesized novel Gelatin-Pluronic F127 hybrid hydrogels, thoroughly analyzing their *in vitro* viability as potential cell barrier membranes for use in GBR. Rheological analysis demonstrated high mechanical strength as hybrid hydrogels' elastic moduli drastically increased with increasing percentages of the chemical cross-linker microbial transglutaminase (mTG). The surface of the hybrid gels was visualized with laser microscope to show topographic changes among different crosslinking density. Cytotoxicity tests were first conducted to show the biocompatibility of hybrid gels. To investigate levels of cell adherence, confocal microscopy was performed on hybrid hydrogels plated with human dermal fibroblasts, which demonstrated significantly reduced cell attachment as compared to pure gelatin. Cell impermeability was further investigated by observing cell migration from gelatin gel to hybrid gel compared with from gelatin to gelatin, with a control setup consisting of Gelatin / Gelatin / Gelatin and an experimental setup of Gelatin / Hybrid / Gelatin. Human dermal fibroblasts plated on gelatin gels migrated through the middle gelatin, but, particularly at the highest mTG concentration, were unable to migrate through middle hybrid gels, showing hybrid hydrogels' impermeability to cells. Our findings, identifying in vitro high mechanical strength, cell impermeability, and biocompatibility, point to novel Gelatin- Pluronic F127 hybrid hydrogels as promising biomaterials for use as GBR cell barrier membranes in treatment of periodontitis.

[1]Bhatnagar, Divya, et al. "Rheological characterization of novel HA-Pluronic thermoreversible hydrogels." *Journal of Chemical and Biological Interfaces* 1.2 (2013): 93-99.

SESSION BI01.08: Sustainability and Materials for Construction, Ceramics and Polymers

10:45 AM BI01.08.02

A Novel Fire Retardant Solution to Mitigate the Onset of Wildfires <u>Yuan Xue</u>¹, Xianghao Zuo¹, Joshua Vilkas², Pik Hoi Lam³, Nicole Jacobsen⁴ and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Hebrew Academy of Nassau County High School, Uniondale, New York, United States;

³Wilson Area High School, Easton, Pennsylvania, United States; ⁴Plainedge High School, Massapequa, New York, United States.

The dangers of wildfires are brought to attention as they frequently ravage wooded areas like California and Greece. The current resolution is reactive rather than preventive, and involves dropping chemicals after the start and expansion of the fire. Additional concerns include the application of non-eco- friendly ingredients to quench the fires. The goal of this research is to engineer aqueous solutions that are sprayed onto leaves prior to the onset of fires to inhibit fires from spreading uncontrollably. Here we describe the results of a formulation that was used on the leaf species, *Cornus kousa*, a subspecies of the *Cornus*, or Dogwood family.

The experiments were conducted on three categories: fresh picked leaves, oven-dried leaves, and naturally fallen leaves. FTIR analysis of the leaves indicated that fresh leaves consisted of water (2/3 of the mass) while the dried leaves were predominantly of cellulose. Fresh leaves were coated with a thick waxy layer, while the drying process removed some of the surface wax. Different solutions were first formulated where contact angle goniometry was used to optimize the wetting properties for both dry and fresh leaves and viscometer was used to determine the optimal viscosity for spray applications.

The solutions were then applied by spraying onto fresh leaves and piles of dried leaves. Burning tests were performed both on leaf piles, and individual leaves, using a propane torch. The flame was applied continuously for five seconds and then removed, and the time to self-extinguish was recorded together with the extend of the spread of the fire.

Results indicated that for fresh leaves, in the absence of the spray, the fire persisted till at least ³/₄ of the mass was consumed and for the dried leaves the entire mass was consumed before the fire was removed. With the addition of the spray, the fire self-extinguished immediately after the flame was removed, and the fire during the application of the flame consumed less than 25% of the mass. Similar results were obtained for both wet and dry leaves. FTIR and RAMAN spectroscopy was performed at each stage in the testing in order to determine the underlying mechanism leading to the flame retardant properties.

The toxicology of the solution and the individual components is being tested on grass and vegetable plants. Preliminary data, thus far, had not found any significant differences in root size or germination rate between the control plants culture and those watered with the undiluted solutions. The results of ongoing experiments regarding sequestration of the chemicals in the leaves and fruits will be presented.

SESSION BM01.03: Poster Session: 3D Printing of Passive and Active Medical Devices

1:30 PM BM01.05.01

In Situ X-Ray and Thermal Characterization of FDM 3D Printing <u>Yuval Shmueli</u>³, Jiaolong Jiang³, Thomas Howell³, Ellen Wachtel¹, Gad Marom², Dilip Gersappe³ and Miriam Rafailovich³; ¹Weizmann Institute of Science, Rehovot, Israel; ²The Hebrew University of Jerusalem, Jerusalem, Israel; ³Stony Brook University, The State University of New York, Stony Brook, New York, United States.

Fused deposition modeling (FDM) printing is an emerging 3D printing technology in which thermoplastic filaments are extruded and deposited in certain manner according to computer input design. FDM is a rapidly developing new area where new methodology is required to explore phenomena far from equilibrium. In this study, we use *in-situ* synchrotron X-ray scattering and high resolution infra-red imaging to study in-situ the relationship between the extrusion parameters, the filaments deposition directionality and the internal structure of the nanocomposite. In two steps study we place first "home-made" extrusion setup and then open-walls 3D printer in the beamline.

The results are then compared with Lattice Boltzmann Modeling which simulates the welding between filaments as a function of nozzle parameters, printing protocols, and the system thermodynamical response function. In filled systems, using in-situ X-rays scattering, we observed the effect of extrusion shear forces on the orientation of the nanoparticles and the influence of the particle/polymer interactions on the polymer crystallization. This phenomenon ("Transcrystallization") leads to templating of the polymer crystalline structures by the fillers which, we show, can enhance the thermal, mechanical and electrical properties of the printed nanocomposite structures, under directional control by the printing algorithm. The results of insitu printing measurements show how the parameters of sample temperature, printing orientation and materials composition affect the internal structure and crystalline structure formation.

We Acknowledge support from the National Science Foundation (Inspire Award No. 1344267) and The Morin Foundation Trust.

SESSION BM04.06: Poster Session II: Biomaterials for Regenerative Engineering

Engineering Titanium Substrate by Atomic Layer Deposition for Dental Pulp Stem Cells Proliferation and Differentiation Studies <u>Ya-Chen Chuang</u>^{1, 2}, Likun Wang¹, Marcia Simon³ and Miriam Rafailovich¹; ¹Materials Science & Engineering, Stony Brook University, The State University of New York, Stony Brook, New York, United States; ²ThINC Facility, Advanced Energy Center, Stony Brook, New York, United States; ³Oral Biology & Pathology, Stony Brook University, The State University of New York, Stony Brook, New York, United States.

Stem cells are sensitive to both chemical and mechanical changes in the environment, which proliferation and differentiation depend on three main factors: the type of stem cell, the underlying scaffold, and the signaling molecules added. It has been shown that stem cells isolated from the dental pulp (dental pulp stem cells (DPSCs)) can differentiate and express markers of odontoblasts, osteoblasts, adipocytes or neuronal cells when they are grown in specific inducing media. However, the external chemical inducers such as steroids can cause adverse side effects such as hyperglycemia and a weakened immune system in clinical studies. Therefore, we focus on engineering the underlying substrates to induce DPSCs differentiate along the desired pathway without external chemical inducers added. Titanium, a material used as dental implant, has shown to promote its osseointegration with specific surface treatment to manipulate its surface roughness and topography. Herein, we introduce a new method to fabricate titanium substrate by atomic layer deposition (ALD), which deposits a homogeneous 2~3nm thickness of titanium on silicon wafer substrates. Due to surface chemistry changed, DPSCs have shown to proliferate well on ALD titanium substrates compared to bare silicon surface. At week 4, biomineralization were characterized by SEM/EDS and Raman

spectroscopy. RT-PCR was also used to identify odontogenic and osteogenic differentiation markers. The results showed that biomineralized deposits (Ca/P) along with collagen fibers were observed on ALD titanium substrates, and RT-PCR results showed that osteocalcin (OCN) was upregulated from week 2 to week 4 but Dentin Sialophosphoprotein (DSPP) expression remained low over 4 weeks. It suggests that DPSCs growing on ALD titanium surface might induce them to differentiate along osteogenic pathway.

The ALD method provides a fast and easy process to coat a homogeneous thin layer of titanium on the substrate, where only surface chemistry changes but which roughness and topography remain the same. This method could be a potential application to coat a thin layer on titanium on any biomaterial to further promote stem cells differentiation and proliferation. [We would like to thank the NSF-INSPIRE program (Grant #1344267).]

BM04.09.10

Synthesis and Characterization of Non-Cell-Adhesive Gelatin/Pluronic Hybrid Hydrogels Juvi Li, Clement Marmorat, Miriam Rafailovich and Marcia Simon; Stony Brook University, Stony Brook, New York, United States,

Non-cell-adhesive biohydrogels stand important roles in many in vivo applications. In the case of periodontitis, a biohydrogel non-cell-adhesive material could isolate the soft gum tissue from the hard bone and promote selective growth of both tissues on each side of the membrane. Many shortcomings are associated with the use of current materials like polytetrafluoroethylene including degradability, workability, cost or cytotoxicity. In this study, we introduce a novel costeffective material, a hybrid biohydrogel of gelatin and Pluronic F127, strong enough to withhold mechanical degradation during the surgical procedure but yet degradable in vivo, non-cytotoxic, porous to promote the diffusion of nutrients and physiological fluids while remaining antiadherent to gingival fibroblasts, would be ideal for this type of application. The hybrid gels were crosslinked via microbial transglutaminase (mTG).

Hybrid gels with different ratio of gelatin, F127 and mTG were synthesized. Rheological properties of those gels were determined by rheometer and the surface and side cut section of those gels were observed by laser scanning microscope and scanning electron microscope. UVvis and FT-IR spectroscope were used for structure characterization of the hybrid gels. Fibroblast with green fluorescent were seeded on the surface of hybrid gels to determine cell adhesive ability. Our results showed the synthesized hybrid gels preserve the mechanical stability of gelatin-based hydrogels, while also exhibiting excellent workability and non-cell-adhesive properties of Pluronic F127.

BM04.09.17

The Effects of Graphene in Different Morphologies of Polymer on Dental Pulp Stem Cells Linxi Zhang¹, Kuan-Che Feng¹, Chung-Chueh Chang², Marcia Simon³ and Miriam Rafailovich¹; ¹Materials Science and Engineering, Stony Brook University, The State University of New York, Stony Brook, New York, United States; ²Advanced Energy Center, Stony Brook University, The State University of New York, Stony Brook,

New York, United States; ³Oral Biology and Pathology, Stony Brook University, The State University of New York, Stony Brook, New York, United States.

Graphene and graphene-based materials have been developed and widely used in tissue regeneration engineering, due to their excellent physical properties. Many studies have shown that graphene can control and accelerate multi-lineage differentiation of stem cells in vitro. Graphene are commonly used, in most studies, as the substrates which have direct contact with cells. In general cells do not interact directly with substrates. Rather, extracellular matrix proteins secreted by the cells adsorb first, coating the substrates, enabling cell adhesion. Hence as was previously shown, the response of the cells on these substrates will depend on the conformation of the adsorbed ECM. Therefore, in order to comprehend the mechanism through which graphene affects stem cell differentiation, it is important to understand the influence of graphene on ECM protein structures. We have previously shown that the differentiation of dental pulp stem cells is greatly affected by the substrate morphology of poly(4-vinylpyridine) (P4VP). It provides a perfect platform to study the the additional effect of graphene on the cells. We found that graphene can be easily distributed into this system by electrospinning and spin coating process.

The cell behavior and biomineralization and differentiation of DPSCs on the graphene-containing scaffolds are determined by multiple techniques, including SEM, Raman and RT-PCR. The results show that the cell-secreted ECM structure and biomineralization on different scaffolds are affected by the addition of graphene in the original polymer matrices. The research was supported in part by the NSF (Inspire Award #1344267) program.

BM04.09.41

Utilization of P4VP and Graphene to Differentiate Dental Pulp Stem Cells into Functional Neurons John Chen¹, Zaiff Khan¹, Linxi Zhang², Kuan- Che Feng², Rebecca Isseroff², ¹, Marcia Simon³ and Miriam Rafailovich²; ¹Lawrence High School, Cedarhurst, New York, United States; ²Dept. of Materials Science and Chemical Engineering, Stony Brook University, The State University of New York, Stony Brook, New York, United States; ³Stony Brook University School of Dental Medicine, Stony Brook, New York, United States.

Currently, the central nervous system is unable to heal effectively by itself, leading to a search for ways to regenerate or grow neurons for replacement. Dental Pulp Stem Cells (DPSCs), easily acquired from extracted wisdom teeth, are multipotent stem cells that can transform into osteoblasts, cardiac, and neuron cells and can thus provide cells resulting in an autologous implant. P4VP, a polymer shown to retain cell morphology, can help cells adhere to a substrate, potentially eliminating the need for polyornithine. Graphene, known for its electrical conductivity, may prove useful in the differentiation of DPSCs into neurons, since neurons communicate through the electrical impulses of the synapses. This research compares the effects of thin film substrates composed of different combinations of P4VP, graphene, and polyornithine; as well as the effectiveness of these substrate combinations electrospun into fibers, on DPSCs and their potential differentiation into neural cells.

Four experimental substrates were created: P4VP and P4VP + graphene thin films, as well as P4VP and P4VP + graphene electrospun into fibers. Two sets of each substrate were created; one set was coated with polyornithine and the other set was not coated. A positive control of tissue culture plastic was also plated with DPSCs.

Optical microscopy displayed that DPSCs grown on flat substrates of P4VP and P4VP+graphene grew into longer cells than those grown in the positive control. In addition, they had formed branches of axiom-like structures from day 14, even without the use of polyornithine, suggesting that P4VP thin films allow cells to adhere on their own to the substrate. However, electrospun fibers did not show differences in cell growth from the positive control. Confocal Microscopy conducted after 21 days of culture confirmed that the cells directly attached to the P4VP and P4VP+graphene substrate had elongated, while the cells not attached were more round, but both types showed high confluency. Also, cells plated on electrospun fiber samples had the same shape and confluency as flat film samples, suggesting that fibers had similar effects as thin films on DPSC growth into nerve-shaped cells. No visible changes were seen with the addition of graphene. Further results were acquired with Scanning Electron Microscopy (SEM) and Real-Time Polymerase Chain Reaction (RT-PCR), determining whether the DPSCs were starting to undergo differentiation into neurons and thus showing promise that P4VP can provide a suitable scaffold for neuron cell development.

BM04.09.45

Influence of Exposure to TiO2 Nanoparticles on *Staphylococcus aureus* **Infection** Fan Yang¹, Justin Zhou², Vincent Zhang³, Jonathan Goldschlag⁴, Ethan Winkler⁴ and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Patchogue-Medford High School, Medford, New York, United States; ³Sachem High School East, Farmingville, New York, United States; ⁴Hebrew Academy of the Five Towns and Rockaway, Cedarhurst, New York, United States.

Titanium dioxide (TiO₂), commonly used in paints, toothpaste, sunscreen, cosmetics, pharmaceutics, and food additives, has been extensively studied for its anti-cancer and anti-bacterial applications when irradiated with UV light, but there is minimal data on its relative safety for normal human cells. In a previous study, HeLa cell exposed to TiO_2 nanoparticles showed an increased susceptibility to bacterial infection partially attributed to inhibition of enzymatic activity involved in membrane cholesterol distribution.[1] Since HeLa cells are an

immortalized cell line derived from tumor tissue, they may not be representative of cells found in healthy human tissue. To investigate the influence on healthy tissue, we chose to focus on skin tissue, since skin is the first barrier to contact with various toxins. Dermal fibroblasts and keratinocytes were plated on tissue culture plastic for 24 hours and then exposed for another 24 hours to 0.1 mg/ml of TiO₂. The results indicate that an increased susceptibility to bacterial infection is also present in healthy primary tissue cells.

Since cells are also influence by their environment, we also investigated the role of the substrate on the toxicity to TiO_2 particles, as well as bacterial infection. Preliminary results indicate increased toxicity of the particles, when the cells are cultured on gelatin, and in particular collagen, which is commonly present in the skin tissue.

[1] Xu, Yan, et al. "Exposure to TiO₂ nanoparticles increases *Staphylococcus aureus* infection of HeLa cells." *Journal of nanobiotechnology* 14.1 (2016): 34.

BM04.09.47

Characterization of Thermoreversible Hydrogels from Multiblock Poloxamers and Hybrid Hydrogels for an Application as Cell Barrier Layer Juyi Li¹, <u>Erica Inyoung Choi</u>³, Christina Tong² and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Fairview High School, Boulder, Colorado, United States; ³St. Paul's School, Concord, New Hampshire, United States.

Periodontitis is a highly prominent issue in dental health today and the current solutions such as Guided Bone Regeneration (GBR), or the use of a barrier membrane to separate the alveolar bone and gums, have many shortcomings. These barrier layers can be composed of hydrogels, 3D cross-linked polymeric networks that are used for regenerative medicine; hydrogels are showing very promising applications in the biomedical field due to their biocompatibility and unique properties. Our previous work showed a promising hybrid gel synthesized with gelatin and poloxamer F127. Polymerized multiblock poloxamers maintain the thermo-reversibility but with an improved mechanical property. This study focused on characterization of the multiblock poloxamers PF127, PF108, and PF98 and synthesis/characterization of hybrid gels using these poloxamers to evaluate their potency. Rheology was used to characterize the poloxamer solutions and hybrid hydrogels, revealing that PF108 had a significantly higher elastic modulus compared to the other gels. The laser microscope imaging showed a unique, branching fiber structure of the PF108 hybrid gel, while the structures of the other hybrid gels displayed gelatin mesh networks. The PF108 hybrid hydrogel also showed significantly lower surface roughness. This is associated with decreased cell attachment, thus, gelatin-PF108 hybrid gel may possess promising characteristics to serve as a better cell barrier layer.

[1]Jiang, Jun, et al. "Rheology of thermoreversible hydrogels from multiblock associating copolymers." *Macromolecules*41.10 (2008): 3646-3652.

SESSION BM05.04: Poster Session: Advanced Manufacturing Technologies for Emulating Biological Tissues Session Chairs: Guohao

Engineering a Synthetic Analogue to the Nucleus Pulposus for Spinal Disc Repair Therapies <u>Juyi Li</u>, Clement Marmorat, Yeshayahu Talmon, Raphael Davis and Miriam Rafailovich; Stony Brook University, Stony Brook, New York, United States.

The role of synovial fluids is to enable frictionless motion of joints and provide shock absorbance within the spinal cord for the central nervous system. Injury, disease, and even aging can degrade the structure and mechanical response of the fluid. Here we report on engineering a substitute for the nucleus pulposus, the viscous fluid within the spinal cord discs. Herniation of lumbar discs is a painful condition, which often requires surgical intervention, where the nucleus pulposus is removed and the disc space is fused. Recently hydrogels have been proposed as possible replacements. Yet, despite a great deal of effort, several major challenges must be overcome; The materials are tough and yet injectable and extremely flexible, biocompatible and yet non-adhesive and resistive to enzymatic degradation. Consequently a variety of chemically cross linked synthetic gels or viscous natural hydrogels have not been successful. Here we report on the use of Pluronic physical gels, which we have successfully bioprinted, injected, and shown to prevent scarring and degradation in-vivo in dog trials. The results were very surprising since, despite their tremendous mechanical flexibility, these tri-block copolymers are very sensitive to fluid volume changes. We demonstrate, using SEM microscopy on gel cryo-sections, together with in-situ xray analysis, that in addition to the standard parameters defining the equilibrium state, the stability of physical gels is dependent on the dynamical aspects of the fluid medium. Using a specially constructed flow chamber, we show that for a Pluronic F127 physical gel, the degradation process can be greatly reduced under high fluid flow rate tangential to the gel surface. Since the physical gel is formed by an ordered crystal of micelles, stabilized by entanglements within their coronas, a simple model is proposed where swelling can occur only when the flow rate is less that the reptation time. Otherwise, rather than dissociating into individual micelles, the micelle gel responds collectively to the surface shear forces as an elastic solid, which deforms in a direction perpendicular to the flow in order to minimize stress. This aspect of the Pluronic triblock copolymer system greatly extends their application from an injectable drug delivery carrier to a structural component which is at once injectable, and yet able to sustain deformation and resist dissolution in physical fluids.

[1] Bhatnagar, Divya, Miriam Rafailovich, and Raphael Davis. "Methods Useful in Optimizing the Treatment of Neuropathies and Targeting Tissues with Cosmetic Botulinum Injections." U.S. Patent Application No. 13/463,766.

SESSION BM07.13: Biosensors—Performance

4:00 PM BM07.13.05

Chip-Based Potentiometric Sensor for Flavivirus Diagnostic Using 3D Surface Molecular Imprinting Vincent Ricotta³, Yingjie Yu³, <u>Nicholas Clayton</u>³, Ya-Chen Chuang³, Yantian Wang³, Steffen Mueller¹, Kalle Levon², Marcia Simon⁴ and Miriam Rafailovich³; ¹Codagenix Inc, Farmingdale, New York, United States; ²Chemical and Biological Sciences, Polytechnic Institute of NYU, Brooklyn, New York, United States; ³Materials Science and Chemical Engineering, Stony Brook University, The State University of New York, Stony Brook, New York, United States; ⁴Oral Biology and Pathology, Stony Brook University, The State University of New York, Stony Brook, New York, United States.

The latest Zika virus (ZIKV) pandemic caused great international concern from explosively proliferating throughout the Americas. This arbovirus is primarily transmitted through the bite from an infected mosquito, but infection has also been spread through perinatal transmission, sexual contact, blood transfusion, and physical contact. Although asymptomatic, ZIKV became a

major health crisis due to the link with the steep rise in cases of microcephaly and Guillain-Barré syndrome with infection. With no viable vaccine or reliable and economically feasible diagnosis in sight, the World Health Organization has called for the rapid development of flavivirus diagnostics. Unfortunately, antibody-based detection systems can result in false positive results and RNA-based detection systems are costly, time-consuming, and impractical for testing in remote regions. In this study, a potential point-of-care (POC) diagnostic system was developed using a chip-based potentiometric sensor to detect flaviviruses using a 3D molecular imprinting technique. The co- adsorption of ZIKV and alkanethiols formed a crystalline self-assembled monolayer (SAM) on the surface of the gold chips. The crystalline SAM behaved as lock-and-key complexes by forming cavities on the surface of the chips specific to the size and confirmation of the targeted virus. Re-adsorption of the targeted ZIKV to the cavities yielded surface charging on the chips which was measured in real-time potentiometrically. The formation of these crystalline SAM was verified using cyclic voltammetry. The removal and re-adsorption of the targeted virus was verified using electrochemical impedance spectroscopy supporting the molecularly wired mechanism. This chip-based potentiometric sensor system was able to detect 10⁻¹ PFU/mL ZIKV in a buffered solution under 20 minutes without any sample manipulation. This sensor was tested against Dengue virus at clinical viral loads and showed no sign of cross-reactivity. When tested against human saliva samples containing clinical viral loads, this sensor was able to detect 10 PFU/mL ZIKV among the pool of bio-macromolecules. The high sensitivity and high selectivity demonstrated here proved that this lab-on-a-chip diagnostic has the potential to become a POC detection system for rapid and accurate screening of flaviviruses. This work was supported by the NSF, Inspire #1344267. This work was performed in part at the Advanced Science Research Center NanoFabrication Facility of the Graduate Center at the City University of New York.

SESSION BM07.14: Poster Session III: Bioelectronics—Fundamentals, Materials and Devices

BM07.14.05

Testing the Viability and Reusability of Hemoglobin Biosensors Utilizing SAM Surface Molecular Imprinting and Natural Surface Roughness Indices <u>Yehoshua Auerbach</u>¹, Nicholas Clayton², Miguel Hulyalkar³, Andrew Todt⁴, Rebecca Isseroff², ¹, Vincent Ricotta² and Miriam;Rafailovich²; ¹Lawrence High School, Cedarhurst, New York, United States; ²Dept. of Materials Sciences and Chemical Engineering, Stony Brook University, The State University of New York, Stony Brook, New York, United States; ³South Side high School, Rockville Centre, New York, United States; ⁴Lake Oswego High School, Lake Oswego, New York, United States.

We have shown that molecular imprinting (MI) technology, together with potentiometric detection, can be used to produce sensitive, yet robust, biosensing systems with real-time electrochemical readout that can be utilized for point of care diagnostics. Real time detection of biomarkers is essential when rapid, critical decisions need to be made, such as during medical procedures when cancer is suspected, or when public health is threatened, as in the recent Zika virus epidemic or in dealing with a suspected attack by biological agents. The biosensor that we developed was tested against standard methods, such as ELISA, and was found to have comparable or better sensitivity, with sample sizes which were at least an order of magnitude smaller. Furthermore, the results from the technique are obtained within minutes, using inexpensive potentiometric readout technology which can even be wirelessly transmitted.

These biosensors utilize surface molecular imprinting of a self-assembling monolayer (SAM) of hydroxy-terminated alkanethiol chains that are able to form a crystalline 'lock-and-key' structure around a target analyte; this allows the sensors to detect and differentiate between biomacromolecules of similar size and shape with high selectivity and sensitivity. Therefore, they can be used as a quick yet accurate analysis of many chemical and biological processes, such as stem cell differentiation. The sensors are also very versatile, and can be used to detect molecules with sizes ranging over several orders of magnitude, and of widely varied chemical composition and structure.

In order to fully exploit the advantages of these biosensors, especially in remote, economically disadvantaged areas, it is important to understand and quantify the durability and reusability of the sensors. Polished and unpolished biosensor chips were created to A) test the viability of hemoglobin detection using molecular imprinting techniques, and B) to test if these sensors can be washed and reused after adsorption testing. The successful readsorption of hemoglobin even after washing indicates that these biosensors can be reused, extending the life and usefulness of the device. Further work is in progress to determine the number of uses for the device, and the optimal method for storage. Preliminary work seems to show that vacuum sealing of the sensors with a commercial device is adequate, indicating that convenient long-term packaging of the sensor can be achieved, in turn enabling shipping and storage.

SESSION ET03.03: Poster Session I: Electrocatalysis

ET03.03.05

Graphene Oxide Enhanced Performance and Durability of Proton Exchange Membrane Fuel Cells (PEMFCs) <u>Likun Wang</u>¹, Yuchen Zhou¹, Stoyan Bliznakov¹, Miriam Rafailovich¹, Danielle Kelly², Audrey Shine³ and Guan Hao Chen⁴; ¹Stony Brook University, Stony Brook, New York, United States; ²Friends Academy, Locust Valley, New York, United States; ³Plainview Old-Bethpage JFK High School, Plainview, New York, United States; ⁴St. Georges High School, New York, New York, United States.

Proton exchange membrane fuel cells (PEMFCs) has attracted tremendous attentions as energy conversion device due to its high energy density, low operating temperature and environmentally friendly emission. Numerous efforts have been made to explore efficient catalysts for the reaction when valuable progress brings the large-scale commercialization of PEMFCs to the table. However, durability of the PEMFCs hindered the commercialization process. Here, we reported a simple, low-cost and readily scalable method to mitigate this effect by the incorporation of graphene oxide (GO). In our study, GO is deposited on the Nafion membrane or into the catalysts layer. The maximum power output of the cell under H₂/air atmosphere showed an enhancement over 20%. More importantly, the durability of PEMFCs was significantly improved by the GO introduction. 26.1% of maximum power degradation was observed for the cell without GO while only half amount decrease obtained for the cell with GO after 30K cycles of accelerated stress test based on DOE2020 protocol. Nearly 100% enhancement for the durability of PEMFCs can be attributed to the prohibition of H₂O₂ production. The promising durability promotion effect induced from low-cost GO involvement will help to accelerate the large-scale commercialization of PEMFCs.

SESSION ET04.06: Poster Session II

CM02.03.15

Enhancing Impact Resistance of Polymer Blends via Self-Assembled Nanoscale Interfacial Structures <u>Xianghao Zuo</u>, Yuan Xue, Yichen Guo and Miriam Rafailovich; Stony Brook University, Stony Brook, New York, United States.

We have designed and engineered ternary polymer blends with the mechanical properties

comparable to high impact resistant conventional polymers under the guidance of the lattice selfconsistent field model. Tow formulas were used to study the mechanical properties. In one system, poly (methyl methacrylate) (PMMA) was used as the compatibilizer for the widely studied biodegradable polymer blend, poly (lactic acid) (PLA)/Poly (butyleneadipate-co-butylene terephthalate) (PBAT) blend. We characterized the compatibility of those components and found PMMA was miscible with PLA and partially compatible with PBAT, which allowed it to selfassemble to a nanoscale interfacial layer on the PLA/PBAT interface. This PMMA layer can significantly decrease the interfacial energy and strongly entangle with either PLA or PBAT, resulting in the strengthening of the interface and dramatically enhancement of the impact resistance of the ternary blend. The optimal mechanical performance was achieved when the total PMMA concentration was less than 10 wt %. Higher PMMA content embrittled the blend since the additional PMMA did not contribute to the minimization of the interfacial energy but remained in the PLA phase, increasing the glass transition temperature of the matrix. In the other system, as in our previous study, PMMA is miscible with PLA and PS is totally miscible with styrenic polymers such as HIPS and ABS, therefore, PLA/Styrene Acrylic Copolymers (SMMA) with different styrenic polymers were blended during the study. SMMA will self-assemble to become an interfacial layer on the PLA/PS (or HIPS or ABS) interface at very low concentration (SMMA concentration less than 2%), and enhance the impact resistance of the ternary blend up to 50% compared to the binary blend of PLA/styrenic polymers. Increasing the SMMA concentration will form a third phase domain in the polymer matrix which will embrittle the whole system.

ET04.06.03

Enhancing Power Conversion Efficiency and Charge Carrier Lifetime of Metal Halide Perovskite Solar Cells via Insulating Polymer Induced PbI2 Passivation <u>Yuchen Zhou</u>¹, Likun Wang¹, Yifan Yin¹, Zhenhua Yang¹, Chang-Yong Nam² and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, New York, United States.

The metal halide perovskite solar cells (PSCs) with remarkable power conversion efficiency (PCE) have been unprecedentedly popular in the research community in past several years. The state-ofart PSCs require a smooth and pinhole-free perovskite layer. It has been proved that key characters of high- quality perovskites can be obtained through optimizing the kinetics of nucleation and growth of perovskite crystals. Despite of several successful practices of modifying the crystal formation process, the lack of precise controls over the structure makes these methods less repeatable. In this study, we utilized a simple but effective doping method by firstly introducing a small amount of insulating polymer of poly (lactic acid) (PLA) into the perovskite layer as a dopant. The benefits of doping PLA polymer came in 2-folds: 1) the PLA additive can serve as heterogenous nucleus for preferential formation and growth of perovskite crystals in 2D direction; and more importantly, 2) PLA can also introduce PbI₂ passivation via the bonding of electron donor -acceptor pairs between C=O and Pb²⁺. The bonds induced precipitation of PbI₂ would preferentially assemble at grain boundaries of perovskites during the process. It is believed that the passivation of controllable amount of PbI₂ at the boundaries can largely reduce the defects and trap states and benefit the overall cell efficiency. Characterizations based on x-rays diffraction and scattering (XRD and GIWAXS), microscopes (scanning electron microscopy and atomic force microscopy) and spectrometers (photoluminescence emission and lifetime decay spectrometer) were carried out to probe the morphology, structure and optical variation of the doped/passivated perovskites. Doing so, we were able to confirm the increase of crystal grain size, the presence of PbI₂ passivations and the extended charger carrier lifetime, etc, of our passivated perovskites. Finally, as compared with the original counterparts, the non-encapsulated devices of passivated perovskites were able to obtain 20% PCE enhancement when measured under the ambient

condition, with the best PCE exceeding 18%. (This work was supported by the NSF, Inspire #1344267)

SESSION ET04.14: Interfaces, Film Formation and Transporting Materials

2:00 PM ET04.14.03

Enhancement of Film Quality and Photovoltaic Performance of Organic-Inorganic Halide Perovskite via Polycaprolactone Polymer Dopants Induced Heterogenous Nucleation and Defects Passivation Yuchen Zhou¹, Yifan Yin¹, Anisa Prasad², Sirina Prasad², Aum Upadhyay³, Thomas Chen⁴, Byron Phan⁵, Chang-Yong Nam⁶ and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Staples High School, Westport, Connecticut, United States; ³Interlake High School, Bellevue, Washington, United States; ⁴Mission San Jose High School, Fremont, California, United States; ⁵Hunter College High School, New York, New York, United States; ⁶Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, New York, United States.

Organic-inorganic halide perovskite solar cells (PSCs) have been considered a viable member of next generation photovoltaics, which can address the scalability changes with a low-cost solution process. The perovskite layer is the main source of photogenerated electron-hole pairs in PSCs. The energy lose in the hybrid system has been approved to be principally caused by traps at grain boundaries and surfaces as well as point defects such as interstitial defects or vacancies in the perovskite compounds crystal lattice. Therefore, the premier concern in PSCs is constructing a highly crystalized and defect-free perovskite thin film with full surface coverage, smooth, and ordered crystallites with big crystal grains. In this study, we observe a significantly enhancement in power conversion efficiency (PCE) of photovoltaic device by incorporating a small amount of polycaprolactone (PCL) into the perovskite layer. The long-chain PCL polymer can serve as an efficient passivating agent in the bulk film, due to the formation of weak coordination bonds between Pb²⁺ and the O in the ester group of PCL. Furthermore, the PCL polymer with small volume can participate in the nucleation step as heterogenous nucleus and help reduce interfacial energy, which eventually promotes the growth of each crystal grain. As evidenced from the surface scanning electron microscopy (SEM) images, the average crystal grain size of the perovskite layer with PCL addition increases significantly, as compared with the PCL free sample. The enhanced absorption intensity from UV-vis spectra after the incorporation of PCL indicates the increase of film thickness as well as the light absorption ability. X-ray diffraction (XRD) results prove the purity and high crystallinity of tetragonal (I4/mcm) MAPbI3 perovskite phase of the PCL passivated perovskites with no sign of PbI₂ peaks, while signal of trace amount PbI₂ are seen on the PCL free perovskite layers. Moreover, provided by steady-state and time-resolved photoluminescence (TRPL) results, addition of PCL increases the emission intensity and prolongs the charge carrier lifetime of the perovskite layer, which largely results from reduced surface/boundary defects/traps as well as minimized corresponding non-radioactive recombinations due to the passivation of the crystal grains by PCL. As a result, the perovskite thin films with proper amount of PCL addition exhibits superb device performance with PCE of the champion device surpassing 18%, indicating a more than 20% enhancement to the original devices. (This work was supported by the Morin Foundation Trust and the NSF, Inspire program #1344267)

SESSION ET05.03: Poster Session I: Fundamentals of Halide Perovskite Optoelectronics

ET05.03.39

Solvent Effects on the Thin-Film Quality and Photovoltaic Performance of Metal Halide Perovskites <u>Yuchen Zhou</u>¹, Yifan Yin¹, Chang-Yong Nam² and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, New York, United States.

The metal halide perovskite solar cells (PSCs) has become one of the most popular types of photovoltaic devices in past 6 years. High power- conversion- efficiency (PCE), panchromatic light absorptions and long carrier diffusion length, etc, makes the PSCs significantly competitive among the thin film solar cells. However, optimal function and performance of the PSCs usually require high quality of a perovskite film with full coverage, low roughness, big grain size and proper thickness, etc. Numerous methods have been applied to make high quality perovskite film, among which, the solution- based spin casting is one of the most vastly used methods. Although different groups have succeeded in making perovskite film using the spin casting, specific conditions such as solvent type, thermal treatment etc, varies largely. Lack of rational comparisons and instructive guidance on the deposition condition selection result in huge difficulty in performing repeatable experiments. Herein, we compare the effect of solvents, co-solvents and their ratios on the quality of the perovskite thin films. DMF and/or GBL are used as major solvents, while DMSO is applied as the co-solvent. Several ratios of DMF/GBL to DMSO from 10:0, 9:1 to 7:3 have been tried to prepare the perovskite precursor solutions. Interestingly, we observe significant differences on crystallinity, morphology and thickness of the thin film made by different types and combination of solvents. For instance, 1) From the XRD data, perovskite deposited from DMF based solution exhibits 10 times stronger crystallinity as compared with samples made from GBL. 2) SEM images indicate that DMF based solution guarantees compact and 2 times thicker films than the GBL ones, while the surface of DMF made layer shows much higher roughness. 3) Reducing the amount of the DMSO in the solution can promote the smoothness of the surface but result in the decrease of the film thickness. 4) Crystals with smaller grain size are observed in samples made from solution without DMSO, while excessive of DMSO content leads to vacancies inside the films. 5) Films deposited from the combined solvents of 90% DMF and 10% DMSO presents best compactness, thickness, smoothness and crystallinity among all other solvent combinations, showing 1.5-2 times longer charge carrier lifetime and superb PCE with the best device exceeding 17%. We attribute the better quality of DMF deposited layers to higher PbI₂ solubility and lower boiling point of the DMF, as compared with GBL. The addition of DMSO slows down the crystal growth rate of perovskite by forming MAI-DMSO-PbI₂ intermediate, guaranteeing larger crystal grain size. While excessive DMSO, which does not participate in the formation of the intermediates, remains in the supersaturated film (before annealing) and causes rupture and vacancies in the film during the vigorous annealing process. (This work was supported by the Morin Foundation Trust and the NSF, Inspire program #1344267)

SESSION NM01.11: Poster Session III Session Chairs: Jeffrey Fagan and Esko Kauppinen

NM01.07.08

Enhancing the Thermal Conductivity of PBAT/Graphene Composites via Applying PLA as a Second Phase Reorganizer <u>Xianghao Zuo</u>, Yuan Xue, Miriam Rafailovich and Yichen Guo; Stony Brook University, Stony Brook, New York, United States.

In this study, we have designed and engineered polymer blends as an improvement of the thermal

diffusion structure for polymer materials. In our system, poly (lactic acid) (PLA) was used as a second phase reorganizer of the Poly (butylene adipate-co-butylene terephthalate) (PBAT)/graphene composites. Two different types of graphene, H-5 and C-750, were used in this study to guarantee the thermal conductivity of the composites. According to the contact angle measurements and the calculation of the interfacial tension between polymers and graphene, we observed that graphene will be more stable in the PBAT phase than in the PLA one. Therefore, in our blends system, PBAT was designed as the polymer matrix, while the PLA was considered as the minor phase with a comparatively lower concentration. Because the size of H-5 (average around 5) is larger than the PLA domain size (around 3), H-5 can disperse perfectly in PBAT matrix and form continuous thermal diffusion paths. With 20% of graphene H-5, the thermal conductivity of PBAT/PLA blend can achieve a 26% enhancement, as compared with the sample without PLA. Moreover, we discovered that the incorporation of C-750, unfortunately, failed in promoting the thermal conductivity of the PBAT/PLA blend. Since the PLA domain size is much larger than the size of C-750 (average around 750 nm), it can hardly help drive the dispersion of the C-750 in a preferential orientation in the PBAT matrix and makes the formation of the thermal diffusion path even harder.

NM01.11.10

Dielectric Analysis of Chitosan-Graphene-Lithium Perchlorate Films at Room Temperature Swathi Somanathan¹, Vinod K. Aswal², Miriam Rafailovich³ and <u>Radha Perumal Ramasamy</u>¹; ¹Applied Science and Technology, ACT Campus, Anna University, Chennai, India; ²Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai, India; ³Materials Science and Engineering, Stony Brook University, Stony Brook, New York, United States.

Use of environmentally friendly solid polymer electrolytes is important for battery technology. This work aims at investigating effect of lithium in chitosan-graphene films which can be useful for energy storage applications. Lithium ion are small in size. Lithium salts conduct electricity under electric field due to the mobile lithium ions which can easily migrate. Chitosan is an abundantly available biopolymer. It has good film forming ability. However chitosan films do not have good conductivity. Graphene-based functional materials have caused great interests in electronic, medical, environmental applications due to its large surface area, high electrical conductivity and high mechanical strength. H5 Graphene was purchased from XG Sciences, USA. The graphene platelets have approximate thickness of 15 nm and length of 5 micro meter. Chitosan solution was prepared by adding 1% (w/v) of chitosan powder, 1.5% (w/v) of acetic acid and 100ml of double distilled water. The solution was stirred for 30-40 minutes to form a transparent thick solution. A part of this solution was transferred to a plastic dish to form a film at room temperature. To proportionate amount of chitosan solution 33, 66 and 100% (weight with respect to chitosan) of lithium perchlorate (LiClO₄) was added. To a part of the

(weight with respect to chitosah) of infinum perchlorate (LiCiO₄) was added. To a part of the chitosan lithium solution 5% of graphene (weight with respect to chitosan) was added. The solution was stirred and heated for 30 min. This solution was poured on a plastic dish and dried at room temperature in order to obtain chitosan–graphene-lithium nanocomposites. The thickness of the nanocomposite films varied between 50-200 micro meter. Dielectric studies such as conductivity, dielectric constant, dissipation factor and impedance were measured using impedance spectrometer. The conductivity ranges from 10-8 to 10-4 S/cm for graphene-chitosan lithium system. The conductivity of chitosan was lowest. In the absence of graphene the conductivity increases with increasing LiClO₄ concentration. Conductivity (at 100 Hz) for Chitosan, Chitosan 33% LiClO₄, Chitosan 66% LiClO₄, Chitosan 100% LiClO₄ films are 6x10-8, 2x10-6, 2x10-4 and 3.5x10-4 S/Cm respectively. Conductivity (at 100 Hz) for Chitosan 5%H5 33% LiClO₄, Chitosan 5%H5 66% LiClO₄ and Chitosan 5%H5 100% LiClO₄ are 3.5x10⁻⁷, 5x10⁻⁵,

 1.5×10^{-4} and 3.5×10^{-5} S/Cm respectively. The conductivity measurements show that incorporation of graphene decreases the conductivity for films with 66 and 100% LiClO₄. This indicates that graphene induces crystallization of Lithium salts thereby reducing the conductivity. SEM image shows that graphene affects the crystallization of LiClO₄. Both LiClO₄ and graphene increased the dielectric constant of the nanocomposites. Dissipation factor analysis showed that the relaxation behavior is affected due to incorporation of graphene. The dissipation was also relatively low (similar to chitosan), indicating that the nanocomposites do not have much heat loss.

NM01.11.27

Capitalizing on the Molybdenum Disulfide/Graphene Synergy to Produce Mechanical Enhanced Flame Retardant Ethylene-Vinyl Acetate Composites with Low Aluminum Hydroxide Loading <u>Yuan Xue</u>¹, Xianghao Zuo¹, Yichen Guo² and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Pall Corporation, Port Washington, New York, United States.

We have engineered a flame retardant ethylene-vinyl acetate (EVA) composite which has the similar mechanical properties as polyvinyl chloride (PVC) and therefore may prove to be an alternative material for cable sheathing. Four composites were studied, EVA with aluminum hydroxide (ATH), EVA with ATH and molybdenum disulfide (MoS2), EVA with ATH and graphene nanoplatelets (GNPs), and EVA with all three components. Tensile testing showed nearly identical results for the EVA/ATH and EVA/ATH/MoS2 compounds, while the EVA/ATH/GNPs compound had higher mechanical properties. The compound containing all three components showed further enhanced mechanical properties, indicating that a synergy was established. This was further confirmed using Scanning Electron Microscopy (SEM) where GNPs were seen to increase the dispersion of the MoS2 and ATH components within the polymer matrix. Cone calorimetry test clearly showed a large decrease in heat release rate when GNPs were added, which was further enhanced by adding GNPs and MoS2 together. Application of the UL-94 test showed that only the compound containing 36 wt% of ATH and 2 wt% each of MoS2 and GNPs can achieve the UL-94 V0 rating.

SESSION NM01.15: Poster Session IV Session Chairs: Naoyuki Matsumoto and Ranjit Pati

Enhancing Thermal Conductivity and Mechanical Performance of PLA/PBAT Blends with Boron Nitride and Graphene <u>Xianghao Zuo</u>¹, Yuan Xue¹, Frederick Nitta², Jinghan Tang³, Vicki Xu⁴ and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Henry M. Gunn High School, Palo Alto, California, United States; ³Mater Dei High School, Santa Ana, California, United States; ⁴Mission San Jose High School, Fremont, California, United States.

Thermal management is critical to the continually growing electronics industry to prevent devices from overheating and losing their functionality. As low- cost, lightweight, and highly versatile materials, polymers exhibit great potential for heat exchange applications, but their low thermal conductivity is a barrier to their effectiveness. Additive fillers are usually added into polymers to help enhancing the thermal conductivity.

In this study, we investigated the thermal conductivity of blends of PLA (polylactic acid) and PBAT (polybutylene adipate terephthalate) with graphene nanoplatelets (GNPs) and hexagonal boron nitride (hBN). It is hypothesized that the thermal conductivity of the PLA/PBAT nanocomposite would be elevated when adding the fillers compared to neat polymer blends. Contact angle measurements between polymer droplets on hBN and GNP layers deposited on a silicon wafers were used to determine the polymers' relative affinities for the fillers. The

calculation of the word of adhesion between fillers and polymers indicates that both hBN and GNP exhibited more affinity for the PBAT phase than the PLA phase, which means the fillers would be interspersed in the PBAT phase. PLA/PBAT blends with various concentrations of hBN powder and GNPs were blended at 180 using a twin-screw mixer at 150 rpm. The thermal conductivity of PLA/PBAT and PBAT blends with hBN alone was tested at the beginning. Slow increase in thermal conductivity with increasing weight fraction of hBN was obtained. To better enhance the thermal conductivity, considering that we have demonstrated that with the larger size of the fillers which meet the size of the domain in the polymer matrix, they will have a better arrangement, we decided to apply Graphene H-5 in the blends to make some new attempts. The results show that as the GNP content of the nanocomposite increased relative to the hBN content, the thermal conductivity increased significantly. Then, the samples were molded into different sizes to test the impact and tensile properties. The mechanical data indicates that although the combination of hBN and Graphene can help increasing the thermal conductivity significantly, it is difficult to maintain the mechanical properties. Therefore, to enhance the thermal conductivity of the polymer blends with relatively high mechanical performance is a new challenge. We did mechanical tests separately with PBAT/PLA/hBN and PBAT/PLA/GNPs and found that hBN can better maintain the mechanical properties. Thus, we tried different ratios of hBN and graphene and kept the total amount of the filler at 30 wt%. The results show that even 3% of hBN can help maintaining the impact toughness at 85.62 J/m, which is pretty high value that meets the demand for most of the applications.

SESSION TP02.03: Poster Session I

NM01.15.72

Enhancing Thermal Conductivity and Mechanical Performance of PLA/PBAT Blends with Boron Nitride and Graphene <u>Xianghao Zuo</u>¹, Yuan Xue¹, Frederick Nitta², Jinghan Tang³, Vicki Xu⁴ and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Henry M. Gunn High School, Palo Alto, California, United States; ³Mater Dei High School, Santa Ana, California, United States; ⁴Mission San Jose High School, Fremont, California, United States.

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