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AND MECHANICS

ESM Today 2017

February 11

1st Floor Lobby EES Building

14th Annual Engineering Science and Mechanics Research Symposium
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Schedule of Events

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* The Art in Science Exhibition will be held in Room 116
Dr. Varadan is a 1969 alumnus of the Engineering Science and Mechanics department and today is a co-founder, inventor and CMO/CTO/CIO of Nanowear Inc at the Penn State Innovation Park. He has held faculty positions at University of Arkansas, Cornell University, Ohio State University and Pennsylvania State University for nearly 39 years. In 2014 Nanowear Inc was founded and is a leading developer of patented, textile-based nanosensor technology with applications in the cardiac, neurological, diabetic and sports medicine/performance diagnostic monitoring markets. Dr. Varadan has concentrated on the design and development of various electronic, acoustic and structural composites, smart materials, structures, and devices including sensors, transducers, Microelectromechanical Systems (MEMS), synthesis and large scale fabrication of carbon nanotubes, NanoElectroMechanical Systems (NEMS), microwave, acoustic and ultrasonic wave absorbers and filters.

Today Dr. Varadan will be discussing the role of his ESM education and research pathways that helped him in his successful career that involved academia, industry, healthcare sectors and entrepreneurship. The focus will be on nanotechnology application in medicine and health care. Recent progress in nanotextile biosensors and mobile platforms developed by Dr. Varadan and his group has resulted in novel wearable health monitoring systems for neurological and cardiovascular disorders. Nanostructured-textile-based dry sensors can provide long-term measurement of a variety of biological information through seamless integration into garments such as undershirts, bra, headband, socks, bed sheets, etc., of daily use. These sensors can function as wearable wireless health-diagnostic systems that are more intuitive to use when combined with state-of-the-art embedded wireless network devices.
## Oral Presentation Speaker List

### Rooms

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Oral Presentations - EES 114
MOLECULAR TANDEM-REPEAT STRATEGY FOR HIGH-STRENGTH ARTIFICIAL PROTEINS

Huihun Jung\textsuperscript{1,2} and Melik C. Demirel\textsuperscript{1,2}

\textsuperscript{1}Materials Research Institute, \textsuperscript{2}Department of Engineering Science and Mechanics, Pennsylvania State University, University Park, PA 16802

Abstract

Many proteins have repetitions in their sequences or structures. Squid ring teeth (SRT) is a protein complex which is in suction cups and it has segmented semi-crystalline morphology with repetitive amorphous and crystalline domains. These native SRT proteins have three major advantages as a material: 1) strength, 2) toughness, and 3) self-healing property. However, a clear relationship between the molecular structure and the mechanical properties of this material remains elusive due to the imperfect equality of unit sequences in native peptide fragments. To prove the fundamentals of material properties in SRT sequences, we propose a new approach for the design and production of synthetic polypeptides that comprise one or more tandem copies of a single unit with distinct amorphous and ordered regions. We produced segmented polypeptides with varying repeat number while keeping the lengths and compositions of the amorphous and crystalline regions fixed. Our artificially modified polypeptides behave like a segmented copolymer whose structure has amorphous and crystalline domains. We demonstrated that mechanical properties of these synthetic proteins could be tuned by modulating their molecular weights. Specifically, the toughness and extensibility of synthetic polypeptides increases as a function of number of tandem repeats. These results suggest that artificial proteins produced by our approach can help to illuminate the genetic fundamentals of structural protein materials.
Figure 1: Tandem-repeat (TR) construction strategy to control the length of synthetic SRT proteins. (A) DNA and protein sequence of the tandem-repeat unit (n=1). (B) The tandem-repeat procedure phi29 polymerase with nicked and circularized template: the presence of both dNTP and methyl dCTP causes random sizes of double-stranded DNA inserts.

Figure 2: Mechanical testing of films made out of three different sizes of TR synthetic proteins: DMA analysis shows that the toughness (inset) and extensibility of synthetic polypeptides increases as a function of protein molecular weight.

REFERENCES

The field of additive manufacturing, especially in regards to three-dimensional (3D) printing, has quickly burgeoned and has revolutionized the designing and manufacturing of parts. This investigation covers a commercial carbon whisker reinforced polylactic acid composite (Cw/PLA) created using a type of 3D printing known as fused filament fabrication. The investigation’s goal lies in experimentally characterizing and modeling the direction-dependent tensile modulus of elasticity of unidirectionally printed composite material. The models assess the degree of anisotropy resulting from layer-by-layer printing and determine the predictability of the measured properties through the use of micromechanical models. Model predictions rely on measured characteristics such as the length and diameter of the reinforcement as well as the constituent volume fractions. Other material characteristics are assumed, such the spherical shape of voids in the matrix and the perfect alignment and bonding conditions of the carbon whiskers. Tensile modulus is experimentally determined using a hydraulic testing system and a scanning laser extensometer. The models and experiments both indicate that the modulus in the 0-deg. printed direction is about twice the modulus in the 90-deg. printed direction. Similarly, the 0-deg. direction is roughly two times stronger than the 90-deg. direction in tension. The tensile elastic modulus in the 0-deg. direction is well predicted by the Cox model, however, both moduli are over-predicted by the Halpin-Tsai model. The tensile modulus and strength of the as-received feedstock lie between the 0-deg. and 90-deg. properties.
Figure 1: Cross section of Cw/PLA showing fibers (white) and voids (black) retrieved using optical microscopy and image processing software.

Figure 2: Scanning electron microscopy image of carbon whisker embedded in surrounding PLA matrix.

References


Acknowledgements

The Dept. of Engineering Science and Mechanics, the Center for Innovative Materials Processing through Direct Digital Deposition, the Composites Manufacturing Technology Center, and the Schreyer Honors College (all at Pennsylvania State University) are thanked for financial support and for making facilities and equipment available for this project. The author also acknowledges Jeffrey Kim for providing photomicrographs and image analysis results of filament and printed unidirectional cross sections as well as Joseph Bartolai and Dr. St. David John for providing vital support to the manufacturing and testing of the 3D printed specimens.
An optimized condition of squeezing a droplet through a narrow constriction
Zhifeng Zhang, advised by Corina Drapaca

Abstract: Models of droplet passing through narrow constrictions have wide applications in science and engineering. In this paper, we report our findings on the minimum impulse (momentum change) of pushing a droplet through a narrow circular constriction. The existence of this minimum impulse is mathematically derived and numerically verified. The minimum impulse happens at a critical velocity when the average surface tension force balances the dynamic pressure force in the flow, the latter being an indication of total loss in the channel. Finally, numerical simulations are conducted to verify these concepts. These results could be relevant to problems of energy optimization and studies of chemical and biomedical systems.

Table 1 Applications of a droplet passing through a constriction.

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A droplet passing through a narrowly constricted channel is one of the most commonly-used soft matter models. It has wide applications in natural and life sciences and engineering, with examples ranging from basic biological investigations to microfluidic cell-based devices to water-oil emulsion systems. A brief overview of applications of this model is summarized in Table 1.

Figure 1 Squeezing a Newtonian fluid droplet through a circular constriction in a rigid channel with sudden contraction and expansion

In the present research, we conducted both analytical and numerical results. Analytically we get the minimum impulse,

$$I_{\min} = \frac{1}{2} \gamma (V_D + V_c) [2 \sqrt{\frac{P_{sur}}{\rho}} (K_E + K_C)] + \text{const}$$

With critical velocity, as,

$$\bar{U}_{CR} = \sqrt{\frac{4G}{(K_E + K_C) \rho \left( \frac{1}{R_c} - \frac{1}{R_D} \right)}}$$
Numerical results by Volume of fluid method was compared in the following figure.

Figure 2 Impulse of droplet passing through a constriction for droplet with surface tension $\sigma_1=50$ mN/m and respectively $\sigma_2=10$ mN/m

References


2 Zhifeng Zhang*, Corina Drapaca, Xiaolin Chen, and Jie Xu; “Droplet squeezing through a narrow constriction minimum impulse and critical velocity”; Physics of Fluids, Under review

Multiple surface-plasmon-polariton (SPP) waves guided by a chiral sculptured thin film (STF) grown on a 1D metallic grating

Sema Erten, advised by Dr. Akhlesh Lakhtakia

Plasmon is the quantum of plasma oscillations in a metal. Surface plasmons propagate guided by the interface of a metal and vacuum. The quantum is called a surface-plasmon-polariton (SPP) when the vacuum is replaced by a dielectric material. When monochromatic light with a specific wave number parallel to the interface is incident on the interface of a metal and a dielectric material SPP waves can be launched. An SPP wave is highly sensitive to the irregularities near the interface. This feature of SPP waves constitutes the basis of many different applications. For over two decades, SPP wave based applications such as chemical and biochemical detection systems and imaging systems have been suggested and studied [1-4]. The main limitation of the SPP wave sensors is that they can detect only one analyte species at a time. The sensing capabilities of such sensors would increase if multiple SPP waves can be launched at the interface of a metal and a dielectric material.

Experimental excitation of multiple SPP waves can be achieved by implementing Kretschmann, Turbadar-Otto, Sarid or grating-coupled configurations [5]. Motivated by the advantages of using grating-coupled configuration to excite multiple SPP waves, an experimental and theoretical research was undertaken to characterize chiral STFs grown on 1D metallic gratings. For this purpose, 1D gold gratings were fabricated by e-beam lithography on Si wafer substrate. Then, 5- and 7- periods thick zinc selenide (ZnSe) chiral STFs were deposited on top of the gratings by thermal evaporation and serial bideposition (SBD) technique [6]. The samples were characterized optically using a custom-made variable-angle spectroscopic system. The optical response of the chiral STF on top of the gold grating structures was modeled using Mathematica.

The reflectance data acquired experimentally can be used to detect the excitation of the SPP waves. When the angular location of reflectance minimum does not depend on the thickness of the chiral STF it is an evidence of an SPP wave. Another indicator of the excitation of the surface wave is at that angular location a value of n can be found that:

\[ k_x^n = \text{Re}(q) \]

where q is the wavenumber, is satisfied a surface wave can be excited as a Floquet harmonic of order n. Wavenumber q can be found by solving the canonical boundary value problem.

The canonical problem was formulated and solved. The wavenumber values were found and the corresponding angle of incidences were calculated. The absorbance spectrums of the chiral STFs on the gold grating were calculated. The transmittance and reflectance spectrums were measured. The graphs showing absorptances for p- and s-polarization state of the light were plotted and presented in Figures 1-2.

The experimental and computational results showed that multiple SPP waves were launched at the interface of chiral STF and the gold grating. This result is of importance for SPP-wave based sensors due to the increase in the sensing capabilities by exciting multiple SPP waves therefore sensing more than one analyte at a time.
Figure 1: Calculated spectrums of the total linear absorptances of the 5- and 7-periods thick chiral STF on 1D gold grating

Figure 2: Measured spectrums of the total linear absorptances of the 5- and 7-periods thick chiral STF on 1D gold grating

References


A Multi-target with Arbitrary Axes Microdrive for Simultaneous Single-Unit Recordings in Freely-Behaving Rats

Myles W. Billard, Bruce J. Gluckman

Single-unit recordings for systems neuroscience approaches requires targeting neuronal populations in multiple diverse brain structures. In many cases, these cell groups are small and significantly separated; reaching them requires high precision along significantly different trajectories. Here we present a microdrive system which adapts existing drive technologies in combination with novel surgical techniques that leverages standard stereotaxic placement, but decouples the targeting from the placement of the drive mechanism. The microdrive body utilizes an open-platform structure. This provides room for multi-site targeting of individually drivable microwire bundles as well as connections for other physiological measurements, such as electrocorticogram and local field potential recordings. The microwire bundles are integrated into a system of tight fitting tube-cannula combinations. Skull-fixed guide cannulas are implanted individually and stereotaxically to provide the correct positioning and implant-to-target depth. The guide cannulas also provide concentric alignment for the bundle trajectories. Our current design allows for eight individual drive axes with 3 mm drive stroke for each bundle. In total, our system supports up to 32 electrophysiological channel connections for continuous recordings in freely behaving rats. A fully loaded microdrive with an electrode interface board together weigh less than 3 g; a complete system which includes an amplifier board and animal head mount weigh approximately 11 g. This design is readily scalable to higher channel, drive, and target count. Currently, the microdrive is being used to study sleep-wake regulatory dynamics and to test the validity of existing mathematical models of the sleep-wake system.
Figure 1: Multi-position, independently drivable microdrive bundles targeting two distinct brain stem nuclei. One axis is vertically aligned, while the other drive axis is angled to avoid the cerebral aqueduct. Electrode bundles are hand-placed using a 3-axis manipulator to help guide placement tubes into skull-fixed guide cannulas. The depth of each bundle is set when the orange body tube meets the top of the guide cannula.

Figure 2: CAD model showing a complete construction of the microdrive system. Each construct contains electrode bundles, a microdrive body, a flexible-spring drive mechanism, an electrode-interface board, and a 32-channel digital preamplifier.
The Cold Spray (CS) process is a solid-state thermal spray process that achieves material bonding through kinetic energy and plastic deformation. In CS, powder particles are entrained in a heated carrier gas stream and accelerated through a de-Laval converging-diverging nozzle. The particles impact the substrate and undergo plastic deformation and mechanical interlocking. Although the bonding mechanism of CS is understood fairly well, researchers face considerable difficulty predicting particle impact and bonding behavior.

Few material models exist for high-strain-rate mechanics, and the few that do exist are constitutive models that rely on experimentally-determined constants [1], [2]. Perhaps more importantly, these constitutive models are only capable of predicting particle impact at strain-rates below 1x10^5 sec^{-1}. Cold spray impact is on the order of 1x10^7 sec^{-1}. While high strain-rate plasticity models, such as the Johnson Cook constitutive model, have been shown to adequately predict bonding and rebound for low to moderate strain rates, JC is not capable of accurately predicting stress response at the high strain rates that occur during CS without correction factors. For these reasons, a thermodynamics-based plasticity model is better suited to predict material plasticity in cold spray. Recently, Preston et.al. developed a thermodynamics-based model that is referred to as the Preston-Tonks-Wallace plasticity model (PTW) [3]. The PTW model is capable of accurately predicting yield stresses at strain-rates ranging from 10^3 to 10^{12} 1/sec [4]. This accuracy comes at the cost of PTW being considerably more complex than other existing constitutive models. Consequently, the complexity of the PTW model has prevented the model from being widely implemented in high-strain-rate simulations.

This research has successfully implemented the PTW model into a user defined subroutine in Abaqus CAE (Abaqus). The PTW subroutine model was written in FORTRAN 77 convention and integrated into Abaqus using a user-defined VUHARD subroutine, which enables the user to model yield behavior and material behavior based upon user-defined state variables. The subroutine finds the PTW flow stress from three state variables: equivalent plastic strain, equivalent plastic strain rate, and temperature. The PTW then calculates and compares the flow stress for the thermal regime and the overdriven shock regime. The thermal regime occurs at low strain rates and is governed primarily by thermally activated dislocation glide. The overdriven shock regime occurs at high strain rate, where strain hardening has little effect. By accounting for both of these regimes, the PTW model is capable of accurately predicting material behavior over a wider range of strain rates. The final subroutine code was validated using published experimental data. For additional validation, identical simulations were run comparing the PTW subroutine to the Johnson Cook constitutive model native to Abaqus.

In conclusion, the PTW constitutive model was able to be successfully implemented into a user subroutine in order to improve simulation of cold spray impact. The PTW model was then applied to single particle impact simulations. Although the PTW model is significantly more complex than current cold spray material models, the PTW may lead to better material prediction capabilities for CS deposition.
Figure 1: Near Yield Response (1x10^7 N) of built-in Johnson Cook (left) and PTW (right)

Figure 2: Experimental results (left) compared to initial PTW results (right)

References

[5] W. Xie and J. Lee at UMASS
Elevated intracranial pressure (ICP) is an extremely dangerous condition for patients who are suffering from traumatic brain injury, hydrocephalus, or related neurological disorders. To make informed decisions when treating patients, clinicians must understand how the body regulates ICP. Mathematical models can aid in this task [1, 2]. In addition to making quantitative predictions, accurate mathematical models can also describe the transition between different qualitative behaviors of ICP. This is crucial, because, for instance, in a pathological case known as Lundberg A-Waves, ICP oscillates between high and low pressures over a long period. This is in contrast to a healthy state, where ICP remains mostly constant with respect to time.

In this paper, we develop a class of mathematical models of ICP dynamics with the intent to explain how a healthy state of constant ICP can transition to the oscillatory case of Lundberg A-Waves. These models are built by applying the balance of mass and the balance of linear momentum to an idealization of the ventricular cerebrospinal fluid (CSF) compartment of the brain. A schematic of this idealized geometry is shown in Fig. 1. After hypothesizing simple pressure- or volume-dependent control mechanisms that govern the rate of CSF production, the model equations take the form of a system of piecewise-linear ordinary differential equations. For each control mechanism, we then describe the analytical methods used to show either existence or non-existence of a limit cycle, i.e. oscillatory behavior in time. A phase-portrait of such a limit cycle is shown in Fig. . Knowing this, we suggest possible clinical interpretations based on this information.
Figure 1: Idealization of the ventricular CSF system, where $m$ is the effective mass of the ventricle wall, $k$ and $\eta$ are the effective stiffness and damping constants of the deforming tissue, and $x$ is its deformation. The intracranial pressure is $P$, $Q$ is the venous blood pressure, $q$ is the volumetric rate of CSF formation, $A$ is the ventricle wall surface area. The effective spring is unstretched when $x = 0$.

Figure 2: Phase portrait of a limit cycle that is present in the physics-based model coupled with a volume-dependent piecewise-linear control mechanism. Lundberg A-Waves are a condition of oscillatory intracranial pressure that is observed clinically.

References


Oral Presentations - EES 116
Parylene-C microfibrous thin films as phononic crystals
Chandraprakash Chindam, advised by Akhlesh Lakhtakia and Osama O Awadelkarim

The propagation of an elastodynamic wave in a periodic medium has interesting characteristics. One of them is the presence of bandgaps. Depending on the periodicity of medium, elastodynamic waves of frequencies in a certain regimes are either attenuated or reflected. Such frequency regimes where there is no transmittance of the wave through the periodic medium are called phononic bandgaps and in these cases the periodic medium is referred as a phononic crystal. The presence of phononic bandgaps makes these periodic mediums suitable as filters with specific applications in RF filters and MEMS.

Thin films can also be envisioned as phononic crystals. One way to achieve periodicity in thin films is by modifying existing thin physical vapor deposition techniques. Thin films of Parylene C with periodic microstructure have been developed [1]. These films comprise parallel and identical microfibers of upright circular-cylindrical, slanted-circular cylindrical, chevronic, and helical shapes. Since the characteristic dimensions of these Parylene-C thin films were found to be in the micrometer range, we refer to them as microfibrous thin films (µFTFs). Towards a larger goal of establishing the multifunctionality [2] of Parylene-C µFTFs, we investigated them as phononic crystals.

We computationally determined the phononic bandgaps of Parylene-C µFTFs by treating them as phononic crystals comprising identical microfibers arranged either on a square or a hexagonal lattice, shown in Fig. 1. The microfibers could be columnar, chevronic, or helical in shape, and the host medium could be either water or air. COMSOL Multiphysics software was used.

All bandgaps were observed to lie in the 0.01–162.9-MHz regime, for microfibers of realistically chosen dimensions. The upper limit of the frequency of bandgaps was the highest for the columnar µFTF and the lowest for the chiral µFTF. More bandgaps exist when the host medium is water than air. Complete bandgaps were observed for the columnar µFTF with microfibers arranged on a hexagonal lattice in air as shown in Fig. 2. The chevronic µFTF with microfibers arranged on a square lattice in water, and the chiral µFTF with microfibers arranged on a hexagonal lattice in either air or water were also found to have complete bandgaps. Thus, with a choice of host and microfiber, Parylene-C µFTFs can be used as isotropic filters. The softness of the Parylene-C µFTFs makes them mechanically tunable, and their bandgaps can be exploited in multiband ultrasonic filters and bulk-acoustic-wave (BAW) filters. Parylene-C µFTFs can be used as alternative to existing BAW devices since the fabrication procedure for the latter is tedious.
Figure 1: (a) Microfibers of upright circular-cylindrical, chevronic, and structurally right-handed helical shapes with their dimensions chosen for numerical results presented here. (b) Square and hexagonal lattices used for the columnar µTF. Unit cells of (c) square and (d) hexagonal lattices used for the chevronic and chiral µTFs, with lattice dimensions $a$ and $b$, the microfiber diameter denoted by $d$. In (d), the angle $\beta = 2\pi/3$ for chevronic µTFs and $\beta = \pi/3$ for chiral µTFs. In (b)–(d), the unit cell is denoted by $\Omega$, the shaded region $\mathbb{A}$ is completely occupied by the Parylene-C microfiber, and the unshaded region $\Omega - \mathbb{A}$ by either air or water.

Figure 2: Band diagrams for the chosen columnar µTF, with the upright circular-cylindrical microfibers of Parylene C arranged on either (a,c) a square or (b,d) a hexagonal lattice, the host medium being either (a,b) water or (c,d) air. Bandgaps are shown unshaded and each is identified by a number inside a circle.

References


Squid-Inspired Self-Healing Proteins: Controlling the Nanocrystalline Morphology
Abdon Pena-Francesch, advised by Melik C. Demirel

Squid ring teeth (SRT) is a semi-crystalline protein complex extracted from the tentacles of the squid suction cups that exhibits a reversible transition from a rigid to a rubbery material and, therefore, can be thermally shaped into any 3D geometry (e.g., fibers, colloids, and thin films). Recently, Next Generation Sequencing in conjunction with high throughput proteomics were introduced to rapidly identify genes that encode for SRT proteins.

The analysis of SRT amino acid sequence across multiple squid species revealed a segmented copolymer architecture with crystalline and amorphous domains. Inspired in the repetitive sequence motif from five different squid species, squid-like synthetic polypeptides are engineered. Using a tandem repeat (TR) DNA assembly method, polypeptides with repetitive crystal-forming and amorphous blocks were expressed with varying total number of repeat units.

The synthetic proteins, assemble into a semicrystalline nanostructure that grants remarkable mechanical, thermal, optical and conductive properties to the material. However, the presence of topological defects in the semicrystalline network has a strong impact in the aforementioned properties, which is a long standing challenge in soft matter physics. The work presented here establishes a clear relationship between molecular weight of synthetic polypeptides, number of repetitive sequence building blocks, topological network defects and mechanical properties. This results in a predictive model of viscoelastic response of SRT-inspired materials as function of the repeat units and crystallite size.

Furthermore, the self-healing properties of SRT-inspired polypeptides are investigated. Due to the semicrystalline nanostructure of SRT proteins and its reversible glassy-rubbery transition, SRT-based materials can be shaped and self-repaired under mild temperature, pressure and humidity conditions. The repairing process causes a local increase in crystallinity due to the partial re-arrangement of β-sheets, which reinforces the nanostructure.

SRT-inspired self-healing synthetic proteins find applications in numerous fields due to their tunable properties and easy processing. As proof-of-concept, we have developed repairable SRT-coated fibers and fabrics capable of enzyme immobilization, SRT-based underwater bioadhesives at least ten times stronger than other natural adhesives capable of reversible underwater adhesion, and SRT nanotextured coatings for wetting and microfluidics applications among others.
Figure 1: Squid Ring Teeth (SRT) from different squid species: a) Todarodes pacificus, b) Sepioteuthis lessoniana, c) Illex argentinensis, d) Loligo vulgaris, e) Loligo pealei, f) Illex illecebrosus.

Figure 2: Self-healing of SRT-based materials. a) dog-bone specimen is cut in half. b) dog-bone specimen after healing process.

References


Acknowledgements

We thank Huihun Jung and Dr. Benjamin D. Allen for their help in molecular biology and protein expression.
Estimation of Hidden Dynamics in Non-Linear Systems for Predicting Sleep-Wake States
F. Bahari, B.J. Gluckman, K.D. Alloway
Engineering Science and Mechanics Department, Penn State, PA-16802, USA

Over the past decade, my laboratory, the Center for Neural Engineering (CNE), has taken a multi-disciplinary approach to investigate the non-linear dynamics of seizures, with clinical relevance to the treatment of epilepsy (Gluckman 2001, Sunderam 2009). Specifically, my project focuses on further understanding of the underlying neurophysiological interactions that renders a normal brain epileptic. Part of the difficulty in developing effective interventions has been attributed to these neurophysiological interactions that are yet to be completely understood. One such phenomenon is the bi-directional coupling between sleep-wake regulation and seizure activity (Schelter 2006, Sedigh-Sarvestani 2012). There is extensive clinical and experimental evidence that links sleep state to seizure generation. Not only is state of vigilance (awake and alert vs. sleep) or more generally brain state affected by epileptic activity, it also confounds any potential pre-seizure signature. Hence it will infinitely complicate any effort towards accurate seizure prediction and detection. To our knowledge, there are no current seizure prediction algorithms that specifically account for the state of vigilance, most likely due to the difficulty of classifying the sleep state based on EEG.

The CNE has established a rodent model of spontaneous epilepsy which translates well to human temporal lobe epilepsy. Our rodents are continuously cabled for EEG, head acceleration, and single cell recordings. We also perform continuous video monitoring. We have overcome the barriers in obtaining accurate measures of the state of vigilance by combining features extracted from the EEG with head acceleration. The states of vigilance are defined as wake and two types of sleep: rapid eye movement (REM) and non-rapid eye movement (NREM). We have also established a robust system to access and chronically record from sleep-regulatory brain structures deeply embedded in brainstem. This will allow us to further understand the neural dynamics involved in sleep transitions and how they are affected in and affect the epileptic brain.

Sleep state is an emergent phenomenon of the brain network. Changes in sleep state depend on the chemical balance of several crucial neurotransmitters, which in turn are controlled by other factors such as the history of previous sleep states (fatigue) as well as environmental inputs (day vs. night, loud noises). Measurements spanning these elements are often too costly -both expensive and highly invasive. Due to advances in computational neuroscience, physiology, and genetics, several groups have published models of the brain’s sleep-wake network (Diniz-Behn 2014). The models are species dependent, high dimensional (10-22 variables) with many parameters, and non-linear. If we could measure all of the variables within these models, we could first validate the models and then utilize them to gain a mechanistic understanding of the brain dynamics throughout transitions. Then we can iterate the model forward and predict future sleep states. However, our first challenge is that some of these variables are hard to measure simultaneously in the same animal –even just to validate the model thus eliminating further invasive measurements- and some are impossible to measure with current technology. To solve this problem, we can dabble in control theory and use the same techniques that are used to make accurate weather predictions today, namely the Unscented Kalman Filter (UKF). The UKF uses the governing equations of the sleep models and any variables in the model that we are able to measure, and reconstructs the remaining, inaccessible, variables (Voss 2004; Schiff 2009).

The second challenge regards the parameters of the sleep model. If the parameters of the model are perfectly suited to our real, partially inaccessible system, then the UKF should reconstruct the remaining variables faithfully and predictions based on the model would be 100% accurate. But of course, there is a gap between computational models developed using (mostly) simulated conditions, and our real and noisy systems (rodents). Therefore, before we can trust the UKF to reconstruct the system, we have to first estimate the true parameter set. To address this challenge we look to nonlinear data fitting literature and borrow the techniques such as Levenberg-Marquardt fitting algorithm which is essentially a combination of “nonlinear least square” and “gradient” methods (Marquardt 1963). Once this algorithm is coupled with the UKF, we can simultaneously estimate all parameters of the model while reconstructing the dynamics of the real system.

In summary, understanding the role of sleep-wake regulation in epilepsy can drastically improve and even change our approaches in proposing effective treatments. We have established a framework to mechanistically study these dynamics by incorporating experimental measurements into physiologically-based mathematical models. Our efforts will introduce new avenues in model validation, as well as improved understanding of network interactions in epileptic and healthy brain. This has been made possible through the integration of techniques from four different fields. Once we validate the predictive performance of our algorithm, we will move forward to incorporate it into algorithms for seizure prediction.
REFERENCES:


ACOUSTIC STREAMING AND PARTICLE MOTION IN SURFACE ACOUSTIC WAVE DEVICES

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Acoustics in microfluidics, often denoted acoustofluidics, is becoming a promising tool for spatial manipulation of liquids and bioparticles in lab-on-a-chip systems. One way of realizing an acoustofluidic system is to actuate a polydimethylsiloxane (PDMS) microchannel acoustically by surface acoustic waves (SAWs) generated on a piezo-electric substrate via so-called inter-digital transducers (IDTs), see Fig. 1. The surface acoustic waves leak energy into the microchannel and create a pressure distribution, which generate second-order effects such as the acoustic streaming and acoustic radiation forces. Though their extensive use for applications reported in the literature, many physical aspects are yet to be depicted in detailed. For example, what are the exact three-dimensional oscillatory pressure and velocity fields generated in such systems? What are the precise acoustic radiation force potentials for suspended particles? What is the precise acoustic streaming flow generated? What is the critical particle size for which particles can be manipulated via the acoustic radiation forces before they feel a dominating drag from the acoustic streaming flow? To answer these questions a large effort have been put in numerical simulations but detailed quantitative experimental data of the full three-dimensional phenomena is still missing leading to most of the numerical analyzes left non-validated.

In this work, we report measurements of the full three-dimensional motion of microparticles undergoing acoustophoresis in a liquid-filled polydimethylsiloxane microchannel driven by a standing surface acoustic wave. The measurements cover sizes of particles for which their motion is dominated by the acoustic radiation force as well as by the viscous drag from the acoustic streaming. The experiments are supported by a numerical model based on a full thermoviscous and Lagrangian velocity-based formulation. The numerical model correctly predicts the critical particle size for which the domination of motion switches between the radiation force and the streaming drag. Further, the numerical model describes the spatial topology of the acoustic radiation potential as well as the acoustic streaming.

We model the fluid using compressible Navier-Stokes equations without making any apriori assumptions about specific flow regimes. We employ a perturbation approach where the solution of the first-order equations is used to calculate the source terms in the time-averaged second-order equations, which are then solved to obtain the acoustic streaming field. Specifically, we employ Lagrangian velocity based formulation to remove existing ambiguities regarding the second-order boundary conditions. Combining information from these two solutions, it is possible to estimate the mean trajectory of particles in the flow. Since the particle motion inside the flow is governed by the acoustic radiation force, $F_{\text{rad}}$, and the hydrodynamic drag force from the acoustic streaming, the velocity of the particles can be obtained using Newton’s second law via a post-processing of the obtained solutions. These numerical results are then validated with the experimental results obtained from the 3D Astigmatism Particle Tracking Velocimetry (APTV), see Fig. 2. Lastly, we also demonstrate a full fluid-structure interaction case concerning the motion of a deformable object immersed inside the microfluidic channel, see Fig. 3. The numerical solution was obtained via an in-house finite element code based on the deal.II finite element library.
Figure 1: (a) Cross-sectional sketch of the SAW-driven device consisting of a lithium niobate substrate and liquid-filled PDMS channel (width $w = 600\,\text{m}$ and height $h = 125\,\text{m}$). The substrate is acoustically actuated via two sets of interdigitated electrodes (IDTs). (b) Sketch of the computational domain $\Omega$ with impedance boundaries and Dirichlet actuation boundary.

Figure 2: Comparison of numerical results with the experimental results obtained via 3D APTV measurements for particle diameter equal to (a) $0.54\,\mu\text{m}$, (b) $1.2\,\mu\text{m}$, (c) $5.2\,\mu\text{m}$, and (d) $7.8\,\mu\text{m}$.

Figure 3: Simulation showing the deformation of a continuous fluid sub-body originally occupying the circular region in frame (a).
Contact Engineering for High Performance MoS$_2$ Transistors
Joseph R. Nasr, Saptarshi Das

Discovery of graphene has invoked a lot of interest in two dimensional (2D) layered materials[1]. These materials offer astounding physical and chemical properties which allow novel electronic and optoelectronic device engineering. Moreover, these materials are electrostatically superior and mechanically robust. For instance, graphene demonstrates exceptional carrier transport, quantum Hall effect, superlubricity and many other intriguing phenomena[2]. However, the absence of a finite bandgap has limits the integration of graphene in traditional transistor technology. This issue has stimulated great optimism in other 2D materials. Among them black-phosphorous, and various semiconducting transition metal dichalcogenides (TMDs) like MoS$_2$, WSe$_2$ etc. are being considered as promising materials for future nanoelectronic integrated circuits. Distinctive advantage of layered materials is the feasibility of stacking and stitching them together both in lateral as well as vertical direction which opens up unique opportunity for material engineering.

MoS$_2$ is a well-know 2D-semiconductor with an indirect bandgap of 1.2 eV and mobility up to 700 cm$^2$/V-s[3]. In this investigation, we study the performance limit of aggressively scaled and back gated MoS$_2$ thin film transistors with the ultimate goal of developing flexible devices for display applications.

The first focus of this investigation is on contacts on 8 to 60 nm thick exfoliated MoS$_2$. At first, we explored one low and one high work-function metal contacts ($\text{Ti } \Phi_M = 4.3 \text{ eV and } \text{Ni } \Phi_M = 5.0 \text{ eV}$. A 20-nm-Au contact was deposited on top as an adhesive and antioxidant layer which also allows easier probing. Fig. 1a), and 1b) show, respectively, the optical image and device schematic used for this investigation. All Ti contacts had large Schottky barriers due to the metal getting oxidized, which creates an intermediate tunnel junction. The device characteristics with Ti contacts are shown in fig. 2a). Ni contacts looked more Ohmic as evident from linear nature of the output characteristics shown in figure 2b. We fabricated MoS$_2$ devices with different channel lengths ($L_{\text{CH}} = 200-500$ nm). The mobility was extracted to be 25 cm$^2$/V-s from the peak trans-conductance ($g_m$). Different oxide thicknesses (20 and 90 nm) were also investigated.

Non-ideal effects on both the top and bottom interface were characterized. For instance, on the top interface moisture (p-type dopant) caused noise in our device characteristics when measure in ambient. This is due to the adsorption of oxygen and water molecules by the MoS$_2$. This effect was eliminated by measuring the devices in a N$_2$ environment which also increased the ON current by an order of magnitude due to threshold shift as shown in the transfer characteristics in Figure 3.

Lastly, we explored three different alternatives to fabricate high quality and reproducible top gated devices (ALD, h-BN, Ionic Liquid). We also benchmarked MoS$_2$ thin film transistors on 20nm and 90 nm SiO$_2$ oxide.
Figure 1: a) Two-terminal MoS$_2$ device using 60 nm Ni contacts with LCH= 250 & 500 nm. Mobility was reported to be 25 cm$^2$/Vs. b) Device schematic of MoS$_2$-based two-terminal devices.

Figure 2: Output characteristics of MoS$_2$ devices, 250-nm channel length and 90-nm oxide: a) 45-nm Ti Schottky barrier contacts. b) 60-nm Ni contacts showing linear behavior.

Figure 3: Effect on ambience: a) transfer characteristics measured in air. Threshold voltage ($V_{th}$) is 4 V. b) when measured in N2, a threshold shift is observed to $V_{th}$ = -3 V which increases the current.

References:


Experimental investigation on the effect of nano-sized core-shell rubber and silica particles on carbon fiber reinforced polymer

Jeffrey J. Kim, advised by Charles E. Bakis

Since the first introduction of carbon fiber reinforced polymer (CFRP) composite in the early 20th century, CFRP has been rapidly advanced and now lives among human society without being noticed too often. Due to its high strength to weight ratio, CFRP are being implemented in air vehicles, automobiles, and even in bridges. One of the existing concerns of CFRP is the susceptibility in the out-of-plane properties, which are matrix dominant, such as mode 1 fracture toughness ($K_{IC}$) and short beam shear strength (SBS). However, nano-sized particles such as core-shell rubber (CSR) and nanosilica (NS) particles have shown improvement in various mechanical properties [1].

The objective of our project was to successfully manufacture nanoparticles added CFRP specimens using a filament winder and to provide experimental evidence of a possible correlation between $K_{IC}$ and SBS. Through the research, we successfully manufactured CFRP, incorporated with NS, CSR, and even mixture of the two nanoparticles, using a filament winder (Figure 1). Step six of the manufacturing process was the most challenging area of all because in the curing step, the coefficient of thermal expansion (CTE) of CFRP kept creating warpage on the specimens. Cutting the fibers on one side significantly reduced the warpage, successfully manufacturing specimens for mechanical testing.

$K_{IC}$ and SBS were experimentally found (Figure 3). The experiment showed that there was indeed a linear correlation between $K_{IC}$ and SBS (Figure 4). NS added and hybrid of CSR and NS added specimens resulted in the highest SBS. However, it was type 1 hybrid system that also induced the highest $K_{IC}$. Type 1 hybrid system, therefore, performed best in $K_{IC}$ and yet also in SBS.

Overall, this project provided data of correlation between SBS and $K_{IC}$, and also better understanding of the nature of nanoparticles in the manufacturing setting. For the future work, the effects of nanoparticles on CFRP could be validated with computational method.
Figure 1: Overview of the filament winder

Figure 2: Manufacturing process of CFRP on filament winder

Figure 3: SBS test

Figure 4: Relationship between SBS and \( K_{IC} \)

References


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Thermally-controlled In-Situ Bioprinting of Composite Bioink for Bone Tissue Regeneration
Kazim Kerim Moncal, advised by Ibrahim Tarik Ozbekol

Abstract
In this research, we present a new composite bioink solution made of collagen type-I, fibrinogen, thrombin (Thr), transferrin (TG), nano-hydroxyapatite (nHA) particles and Pluronic F127 hydrogel loaded with bone marrow stem cells (BMSCs). Furthermore, we combined the bioink with plasmid BMP2 particles to boost differentiation capability of BMSCs into osteoblasts. A thermally-controlled bioprinting unit (TBCU) was used to accurately control the temperature during the flow of the bioink, which was validated using infrared thermography. Cell viability study was performed after bioprinting, 3rd, 5th, 7th, 14th, 21st and 28th days. Although cell viability was impaired during bioprinting, cells were able to recover and proliferate in a week in culture. Scanning electron microscopy (SEM) pictures were taken to show cells in tissue constructs on the 14th, 21st and 28th days. Thereafter, composite bioink solution was bioprinted directly into critical-size calvarial defect on rats in an operation room using the Multi-Arm BioPrinter (MABP). Five weeks later, rats were harvested and micro-computed tomography (µCT) scan was used to assess the new bone regeneration.

Introduction
Three dimensional (3D) scaffolds have been widely used in bone tissue regeneration [1]. Bone tissue scaffolds should be biodegradable, biocompatible, and able to support enough mechanical properties to maintain the structure until new bone tissue forms [2]. Porosity and pore size are specifically important fabrication parameters for ideal scaffold construction in bone tissue engineering [3, 4]. Bone scaffolds need to have fully interconnected porosity because of enhancing the diffusion of oxygen, transportation of nutrients, and recruitment of progenitor cells during new tissue formation [1, 3, 4].

A wide variety of hydrogels, including alginate [5-7], collagen type-I [6-8], fibrinogen [6, 7], and Pluronic F127 [7] have been used in 3D bioprinting for bone tissue engineering. Collagen type-I hydrogel was shown to facilitate substantial bone tissue formation and has the highest gene expression compared to other hydrogels because collagen type-I is the main and the most important organic component of bone tissue extra cellular matrix [7]. In this study, we present a new composite bioink solution loaded with BMSCs for bioprinting of bone tissue construct directly into the critical size calvarial defect on rats.

Results
MABP was placed in a biosafety cabinet to bioprint 3D bone tissue construct using composite bioink solution, where TCBU components were mounted on one of the arms of the MABP. The composite bioink solution was prepared by mixing collagen solution (9 mg/ml), TG, nHA aqueous solution (1:1 (w/w)) (Collagen:nHA), and Thr, respectively. Thereafter, fibrinogen solution (15mg/ml) was mixed with the prepared solution. Then, Pluronic F127 powder was dissolved at 4°C for 15 minutes in the final solution in order to prepare a final Pluronic F127 concentration of 20% (w/v). When Pluronic dissolved homogenously, the bioink solution was then mixed with BMSCs pellet via pipetting the cell concentration of 2 million cells per ml inside the solution. The scaffold architecture had a lay-down pattern of 0° filament orientation with 0.5 mm pore size and 0.5 mm filament diameter for in vitro study. The scaffolds were printed in 14x12x1 mm totally 2 layers (Fig. 1(A)). The solution was extruded using a pneumatic dispenser (Nordson Corp., Westlake, OH, USA) via the TCBU. Cell viability for fabricated plugs, which was made of using same bioink solution expect Pluronic, were tested using the Calcein staining standard method (Fig. 1(B)). Cell viability was calculated as 95.76±1.15% right after bioprinting. 3 days after, cell viability dropped to 85.92±5.9%. Cell viability; however, increased to 93.63±3.39% on day 10 due to the proliferation of cells and maintained a high viability over time until 28th days. SEM pictures showed that plugs were provided optimal conditions for cells to spread and multiply. Cells were able to attach to collagen fibers and deposit their own matrix. In-situ bioprinting process was occurred after opening 5 mm-diameter 2 mm-thick two defects on rat skulls following the anesthesia. As a control group, plugs made of BMP2 and PDGF particles, separately without cells were implanted into defects. Then, the composite bioink solution was bioprinted into defects using a circular toolpath pattern. Thereafter, calvarium tissues were harvested 5 weeks later to obtain bone volume fractions via µCT scanning. Scanned images were imported to Avizo software to calculate bone volume fraction. Qualitatively, both plug and printed BMP2 treatment was generated more new bone formation compared to other groups.
References

Acknowledgements
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Poster Presentations
Multifunctionality of Parylene C microfibrous thin films
Chandraprakash Chindam, advised by Osama O. Awadelkarim and Akhlesh Lakhtakia

Our objective is to develop a multifunctional material. Although products such as printers serve multiple functionalities: copy, scan, print, email, and fax, multifunctionality still remains a rarity in engineering. In a printer, multifunctionality is achieved by a conglomeration of many single-function devices. For a sustainable future, we need to decrease the number of single-function devices, create multifunctional devices, and make them as smaller as possible. Moreover, in current age of miniaturization, the size of sensors and devices is shrinking rapidly and most of the fabrication is achieved via thin film deposition. In the quest for a multifunctional material, here, we make use of existing procedures in thin film fabrication and explore it for different functionalities. Furthermore, to enhance the number of functionalities, we start with a material that already has industrial applications and is explored in research circles.

Parylene C, a chlorinated member of the xylylene polymer family, has been extensively used as a packaging material in industry [1] – electrical insulation coatings in electronics and corrosion-resistant coatings over prosthetic parts. On the research front, it has been used to study biological cells for retinal prosthesis, and cancer studies. Thin films of Parylene C with periodic microstructure were developed [2]. These films comprise parallel and identical microfibers of upright circular-cylindrical, slanted-circular cylindrical, chevronic, and helical shapes [2]. Since the characteristic dimensions of these Parylene-C thin films are in the micrometer range, we refer to them as microfibrous thin films (µFTFs) polymer.

For these Parylene-C µFTFs, the following functionalities were demonstrated. Experimentally, for columnar µFTFs
1. The molecular and microstructural differences with bulk films were established,
2. Wetting characteristics were contrasted with bulk film,
3. Temperature dependence of dynamic storage and loss modulus were identified, and
4. Temperature-dependent charge storage and absorption characteristics were identified.

Computationally,
1. Phononic bandgaps of columnar, chevronic, and chiral Parylene-C µFTFs in either air or water were identified with the microfibers arranged either on a square or a hexagonal lattice
2. Elastodynamic scattering of microfibers was established.
3. Photonic bandgaps of chiral Parylene-C µFTFs in air were identified.

Additionally, the surface energy and relative permittivity were identified for bulk Parylene C.

References
A Coupled Overset Mesh and Hybridizable Discontinuous Galerkin Algorithm

Justin Kauffman, advised by Jonathan Pitt

Coupling an overset mesh method and the hybridizable discontinuous Galerkin (HDG) finite element method enables solutions to be computed for complex multi-physics partial differential equations that also have complex geometrical features. Overset meshes provide generation of high-quality meshes (i.e. for boundary layers) using structured meshes, and are efficient for moving mesh problems without remeshing or cell stretching. The HDG method’s versatility and adaptability allow for straightforward application to new (and even more complex) problems. The goal of this work is to simulate full-scale hydrodynamics problems. To achieve these simulations, necessary building blocks must first be verified and validated.

For traditional finite volume and finite difference overset methods, in order to increase the order of accuracy, a larger stencil is required at the overset interface, and therefore a larger amount of overlap is required between meshes [1]. The proposed overset HDG algorithm is motivated by the work from Galbraith et. al. [2] where the authors developed a discontinuous Galerkin Chimera scheme that did not require a large amount of overlap between meshes.

The work presented here focuses on a form of the Navier-Stokes (NS) equations. The hydrodynamic problems of interest are typically modeled through the incompressible NS equations, since solving the fully compressible equations would provide no additional information about the flow. However, in an overset mesh configuration mass flow is not conserved along the overset interface for a fully incompressible formulation. To alleviate the incompressibility constraint the balance of mass is altered to allow for some ‘pseudo-compressibility’ as demonstrated in Inagaki et al. [3].

The primary fields in this formulation are: the fluid velocity \( \mathbf{v} \), the pressure \( p \), and the velocity gradient \( \mathbf{L} \). The strong form of the pseudo-compressible NS equations is

\[
\mathbf{L} - \nabla \mathbf{v} = \mathbf{0}, \quad \text{in } \Omega, \tag{1a}
\]

\[
\rho \frac{\partial \mathbf{v}}{\partial t} + \text{div} (-\mu \mathbf{L} + p \mathbf{I}) + \rho \mathbf{L} \mathbf{v} + \rho (\text{div} \mathbf{v}) \mathbf{v} = f, \quad \text{in } \Omega, \tag{1b}
\]

\[
\varepsilon \frac{\partial p}{\partial t} + \text{div} \mathbf{v} = 0, \quad \text{in } \Omega, \tag{1c}
\]

\[
\mathbf{v} = \mathbf{g}_D, \quad \text{on } \partial \Omega_D, \tag{1d}
\]

\[
(-\mu \mathbf{L} + p \mathbf{I}) \mathbf{n} = \mathbf{g}_N, \quad \text{on } \partial \Omega_N, \tag{1e}
\]

where \( \Omega \) is the computational domain, \( \rho \) is the fluid density, \( \mu \) is the dynamic fluid viscosity, and \( \varepsilon \) is the pseudo-compressibility factor.

The computational discrete form of system 1 is verified through the method of manufactured solutions and a mesh convergence study. The study utilizes fifth \((k = 5)\) order elements and Backward Euler (BE) time-stepping. Figure 1 shows the magnitude of the velocity and the overset mesh configuration used to demonstrate optimal order \((k + 1)\) convergence for this formulation. Validation has begun on flow around a cylinder and will be compared to the computational work by Turek [4]. The overset configuration utilizes three meshes, second order elements and BE time-stepping. The problem has a parabolic inlet flow and a zero pressure outlet condition. All other boundary conditions in the problem are no-slip walls. Figure 2 shows the solution for the magnitude of the velocity at \( t = 5s \) for a three overset mesh configuration.
Figure 1: Magnitude solution for the hybrid variable, velocity, and the five overset mesh configuration used to obtain this solution.

Figure 2: Magnitude solution for the hybrid variable, velocity, for a parabolic inlet flow around a slightly offset cylinder at \( t = 5s \).

References


Hydration Dynamics of Squid Ring Teeth Protein by Quasielastic Neutron Scattering

Abdon Pena-Francesch, advised by Melik C. Demirel

The interaction between proteins and water molecules plays a key role in defining the structure and dynamics of the system, as well as the physical properties that arise from them. The hydrogen bonded protein network is disrupted by the water molecules upon hydration, resulting in the plasticization of the protein chains. Although major conformational changes between dry and hydrated states can be observed by conventional methods, spectroscopic neutron techniques provide molecular level resolution to understand hydration effects on protein structure and dynamics.

Quasielastic neutron scattering (QENS) is a spectroscopic technique with 1 – 30 Å spatial resolution and pico- to nanosecond temporal resolution that can study molecular dynamic processes such as rotations, localized motions, diffusive motions and relaxations. Due to the large incoherent neutron scattering cross section of hydrogen, QENS has the ability to selectively probe the self-dynamics of hydrogen atoms. Therefore, the use of deuterated water in QENS protein hydration measurements allows for the direct observation of the protein dynamics since scattering from solvent is negligible, making QENS an extremely useful tool for the study of hydration dynamics of biological systems (e.g. in myoglobin, lysozyme, RNA, GFP, silk, casein, etc.).

Here, we studied the hydration dynamics of a recombinant squid ring teeth (SRT) protein by QENS. Squid teeth (SRT) are protein complexes located in the suction cups of tentacles. This structural protein complex has been shown to have excellent mechanical performance (Young’s modulus of 2-4 GPa in wet conditions and 6-8 GPa when dry). SRT proteins have a semicrystalline nanostructure that consists of randomly oriented β-sheet crystalline nano-domains (~ 3nm in size) embedded in an amorphous matrix. The elastic and quasielastic neutron scattering experiments on 18 kDa recombinant SRT protein (Lv-SRT18) presented in this work show an increased mobility upon hydration which is correlated with the protein nanostructure. While dry Lv-SRT18 low mobility dynamics are dominated by localized methyl group rotations, hydrated Lv-SRT18 high mobility dynamics are dominated by the confined diffusion of amorphous chains within the β-sheet nanocrystalline structure. The two dynamic modes are representative of a dry glassy state (where the full protein chain is heavily hydrogen-bonded) and a hydrated rubbery state (where the amorphous segments of the chain are diffusing in between β-sheets crystallites). The findings have implications in the design of novel engineered polypeptides, where the amino acid sequence governs the formation of a semicrystalline nanostructure and restricts the chain mobility (resulting in tunable mechanical, thermal and optical properties of protein materials).
Figure 1: Disc Chopper Spectrometer (DCS) at NIST Center for Neutron Research (NCNR) in Gaithersburg MD. High Flux Backscattering Spectrometer (HFBS) and DCS were used to measure the dynamics recombinant Squid Ring Teeth protein.

Figure 2: Elastic Fixed Window Scans show the mean square displacement, $\langle x^2(T) \rangle$, of dry and hydrated recombinant Lv-SRT18 protein as function of temperature.

References

High energy density electrochemical capacitors that can provide energy storage solution for self-powered energy harvesting platforms were fabricated. The capacitor development was enabled by synthesis of high purity nanocarbon materials. In particular, we focused on developing two different types of electrochemical capacitors that include:

1) Electrochemical double layer capacitors (EDLC)

Charge storage mechanism in EDLC is primarily based on the formation of electrical double layer at electrode/electrolyte interface. Symmetric EDLC capacitors were made using high purity carbon electrodes derived from polymer precursors with surface area > 2000 m2/g that suppressed solvent decomposition and leakage current.

2) Lithium ion Capacitors

Asymmetric design based on the use of a double layer electrode and a prelithiated anode that provides larger cell voltage (> 4V) and high energy density were fabricated. Various carbon nanomaterials are currently being synthesized to push the energy density beyond 300 J/cc.

In this investigation, symmetric capacitors made using the synthesized carbon electrodes in neat 1-butyl 3-methylimidazolium tetrafluoroborate exhibited a specific capacitance of 136 F/g at 1 A/g when charged and discharged between 0 to 3.8V. The capacitor also showed 90% capacitance retention over 5000 cycles.

In order to further evaluate the fabricated capacitor, accelerated floating voltage was conducted. The tests showed that the capacitor retained 80% of its initial value after 55 hours at 3.8V and 90% retention at 3.5V after 260 hours. The maximum gravimetric and volumetric energy density of the capacitor was 74.4 Wh/kg and 37.5 Wh/l, respectively.
Figure 1: (a) Galvanostatic charge/discharge cycling of the capacitor cycled upto 3.8V cycled at 1 A/g and (b) Specific capacitance as a function of current density.

References


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A new aspiration-assisted bioprinting technique for organ printing

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In contrast to traditional two-dimensional (2D) cell culture, three-dimensional (3D) tissue spheroids offer many advantages, such as the ability of cells to secrete their own extracellular matrix (ECM) and increasing effective communication between cells in a particular tissue microenvironment [1,2]. Clinical studies of new drug take years to complete and often cost more than $5 billion [3]. Animal-based test models are currently the primary means for testing new drugs. They are expensive, immoral, and fail to mimic human physiology accurately. Therefore, it is important to investigate alternative methods which provide better means of testing the effects of new drugs and are not only a better representation of the human body, but also can be produced easily at a lower cost [4].

Recently, one of the primary focus of bioprinting research has been the development of various methods to automate the manufacturing process of functional 3D tissue constructs for drug testing. In order to bioprint spheroids, we have investigated a new process, which enables precise positioning of tissue spheroids onto a fibrin scaffold. We have developed an aspiration-assisted bioprinter (ABB), where a pipette, mounted on the arm, picks the spheroids via the aspiration pressure and places them one by one onto fibrin (Fig.1.). Each spheroid is visually inspected before printing onto desired location. The inspection process reduces the chances of contamination and ensures that only the spheroids of desired size and shape are used to construct the tissue. Automatic and semi-automatic control modes implement a rapid process cycle with a variable level of control and process automation.

For spheroid fabrication process we have utilized U-bottom well microplate with cell repellent surface. During the spheroid fabrication it was observed that the relative size of the spheroid depends on cell number, culture time and cell type (Fig.2.). Higher cell concentration correlated significantly (p<0.001) with larger spheroid diameter for both cell types. βTC3 spheroids made with 5k cells displayed an increase in diameter day 2 (522.1 ± 36.85 μm) and day 3 (533.2 ± 26.66 μm), while βTC3 spheroids diameter made with 10k cells decreased significantly between day 1 (795.75 ± 33 μm), day 2 (699 ± 34.41 μm), and day 3 (618.58 ± 31.52 μm). The diameter of the spheroids with 2.5k cells was consistent throughout day 1, 2, and 3 with an average of 400 μm.

In order to demonstrate the ability of ABB bioprinter, we have placed spheroids precisely, through assembly of various complex patterns such as: line and triangle (Fig. 3.) The viability of the control group was determined to be 94.19 ± 2.55%. Spheroids that were picked and placed into cell media were 88.07 ± 2.02%. When printing onto fibrin, the cell viability was measured as 82.53 ± 7.03% (Fig.4.). The decrease in cell viability after both printing procedures could be due to cell damage during placement. The cell viability was lowest after printing onto fibrin possibly because of the density of placement surface, and drying out issue. The viability of this process was higher than the viability of only bioprinting onto fibrin scaffold.

By monitoring spheroids and reducing the handling time we maximize the cell proliferation of the final biostructure. This bioprinting technique has the ability to monitor and maintain required back pressure while capturing and placing the spheroids during their placement. This novel bioprinting technique can be used for...
many organ-on-a-chip platforms for drug screening.

Fig.1. Aspiration-assisted bioprinter (a) bioprinter setup, (b) pneumatic control system, (c) spheroid bioprinting platform, (d) interface of the aspiration-assisted bioprinter

Fig.2. Fabrication of BTC3 and 4T1 spheroids with different cell numbers

Fig.3. Spheroid patterns: (a) line spheroid pattern, (b) triangle spheroid pattern

Fig.4. Cell viability of spheroids before and after bioprinting (a) a confocal image of spheroid before bioprinting, (b) a confocal image of spheroid after bioprinting into cell media, (c) a confocal image of spheroid after bioprinting onto fibrin, (d) a graph represents cell viability before bioprinting, after bioprinting into cell media and after bioprinting onto fibrin

References


Stimulation on stem cells in adult mouse’s rhombencephalon using transcranial focus ultrasound

Jiayang Liu, advised by Bruce Gluckman

Cell genesis occurs in human brains and the human brain retains the potential for self-renewal\(^1\). How to take advantage of this potential is worth of our efforts.

Adult stem cells are undifferentiated cells found throughout the body that divide to replenish dying cells and regenerate damaged tissues. Research into adult stem cells have been fueled by their abilities to divide or self-renew indefinitely and generate all the cell types of the organ from which they originate — potentially regenerating the entire organ from a few cells. Neural stem cells are multipotent cells with the ability to differentiate into neurons, astrocytes, and oligodendrocytes in the developing stage. Unlike embryonic stem cells, the use of adult stem cells in research and therapy is not controversial because the production of adult stem cells does not require the destruction of an embryo. Adult neural stem cells can be isolated from a tissue sample obtained from an adult. They have mainly been studied in humans and model organisms such as mice and rats.

Lineage specification is strongly sensitive to the mechanical properties of the cellular environment. The reason is that mechanically - gated ion channel Piezo1 is expressed by brain derived neural stem cells and is responsible for a mechanically induced ionic current. Piezo1 activation elicits transient Ca\(^{2+}\) influx in a substrate-stiffness–dependent manner, favors nuclear localization of the mechanoreactive transcription coactivator Yap, and influences neuronal vs. glial specification\(^2\).

A rhombomere (Figure. 1) is a transiently divided segment of the developing neural tube, within the hindbrain region in the area that will eventually become the rhombencephalon.

The advancements in FUS (Focused ultrasound) technology enable the transcranial delivery of the acoustic energy to highly-localized areas (on the order of a few millimeters) across the brain, including deep brain structures\(^3\)\(^-\)\(^5\), which provides us a potential tool.

Here, we investigate the transcranial FUS stimulation effect on stem cells in adult mouse’s rhombencephalon through activating the mechanically gated ion channel Piezo1 in stem cells in-vivo non-invasively (Figure.2). We use in vivo BrdU incorporation and detection in mouse\(^6\) to show the stimulation effect (Or use Calcium based imaging method).
References

Electrospun SRT Waveguides for Applications in Protein-based Photonic Devices

Robert Shreiner, advised by Dr. Melik C. Demirel

As biological, programmable building blocks, proteins offer an elegant means through their sequence-structure-property relationship for the design of novel optical materials. In contrast to the rigid, inorganic, and expensive technologies incorporated in current photonic systems, proteinaceous components would allow the realization of flexible, biocompatible, and economical devices, transforming the emergent field’s application sphere. As an elementary component responsible for relaying information throughout optical circuits, protein-based waveguides are among the most important precursors for functional design. Here, for the first time, such proteinaceous waveguides have been demonstrated. Semi-crystalline structural protein, i.e., recombinant squid ring teeth (SRT) from *Loligo vulgaris*, were processed into microfibers through the electrospinning technique (figure 1). Under the influence of large electrostatic fields, protein solution was propelled towards conducting collecting plates, the solvent evaporating en route with microscale fibers subsequently forming. Laser light was then coupled to the fibers, confirming their optical transmission capabilities (figure 2). When considered with the fabrication of additional protein-based optical components (e.g., previously demonstrated SRT whispering-gallery mode resonators), these results suggest proteinaceous materials may open an exciting path for next-generation photonics, revolutionizing the practical design of tunable, soft, and eco-friendly technologies.
Figure 1: Electrospinning apparatus utilized for fiber production (scale bar 0.1 mm)

Figure 2: Coupled light transmitted along recombinant SRT fiber (scale bars 50 μm)

References


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Droplet-based Bioprinting of Fibrinogen and Thrombin for Engineering Native-like Skin Tissue

Hemanth Gudapati, advised by Dr. Ibrahim Ozbolat

Engineering tissues with native-like characteristics is challenging at present [1]. However, droplet-based bioprinting (DBB) precisely places bioink droplets (of dimensions ≥ 10 µm [2] with an accuracy of ± 5µm [3]) and makes the engineering of tissues with native-like characteristics possible. Here, we investigate the bioprintability of the natural protein fibrinogen and its crosslinker enzyme thrombin using DBB modalities such as piezoelectric drop-on-demand inkjet (PIJ) bioprinting and micro-valve bioprinting for engineering native-like skin tissue (see Fig. 1). Fibrinogen and thrombin are found in blood and fibrinogen enzymatically crosslinks into fibrin hydrogel through thrombin and helps in blood clotting for wound healing. Also, fibrin hydrogel can act as extra cellular matrix (ECM) for the bioprinted cells and provide structural support to the cells. Hence, fibrinogen and thrombin are suitable for engineering native-like skin tissue by using them as fibrin hydrogel precursor solutions and depositing the solutions using the DBB modalities.

In our experiments, fibrinogen (10 mg/ml w/v) showed shear-thickening behavior and fibrinogen droplets generation using the PIJ mechanism is difficult and not reliable. On the other hand, thrombin (5 U/ml) showed relatively Newtonian behavior and the droplets generation using the PIJ mechanism is reliable for the thrombin concentrations of 5-15 U/ml. As a result, fibrinogen droplets are produced using the micro-valve mechanism whereas thrombin droplets are produced using the PIJ mechanism for patterning the skin tissue constructs. The micro-valve is actuated by using a unipolar wave (see Fig. 2A1) with an excitation voltage of 5 V and a dwell time of 500 µs and an excitation frequency of 100 Hz. The voltage pulse characteristics do not affect the fibrinogen droplets volume. However, the fibrinogen droplets volume depends on the fibrinogen concentration, the cell concentration and the pneumatic pressure used for driving the bioink from the reservoir to the micro-valve. The PIJ dispenser is actuated by using a bipolar wave (see Fig. 2A2) with an excitation voltage of ± 30 – 35 V and a dwell time of 20 µs and an echo time of 5 µs and an excitation frequency of 100 Hz. The thrombin droplets volume depends on the thrombin concentration, the excitation voltage, the dwell time and excitation the frequency.

Tissue constructs (see Fig 2B) are fabricated by bioprinting alternating layers of fibrinogen solution containing mouse 3T3 fibroblast cells and thrombin solution respectively. The crosslinking of bioprinted fibrinogen depends on the distance between the fibrinogen droplets and the density of cells in it. Also, the fibrinogen crosslinking depends on the volume of the bioprinted thrombin which depends on the characteristics of the voltage pulse used for actuating the piezoelectric actuator as well as the distance between the bioprinted thrombin droplets. Tissue constructs patterned using fibrinogen of concentration 20 mg/ml (w/v) with 1-3 million 3T3 cells/ml and thrombin of concentration 15 U/ml remained intact for as many as seven days. The post-bioprinting viability of the tissue constructs is about 75% after 1 day. The viability of the constructs increased to 95% after 3 to 5 days (see Figs. 2C1-3).
Figure 1: Experimental set-up used for producing fibrinogen and thrombin droplets.

Figure 2: (A1) A unipolar voltage pulse is used for actuating the micro-valve dispenser whereas a (A2) bipolar voltage pulse is used for actuating the piezo-inkjet dispenser; (B) Bioprinted fibrin construct at 0h which remained intact after culturing in cell media for 24 to 72 h; Confocal images of calcein and ethidium homodimer stained cells in the bioprinted tissue construct after 1 day (C1), 3 days (C2) and 5 days (C3) respectively; Lives cells with intact cell membrane are stained green whereas dead cells nuclei with compromised cell membrane are stained red.

References


Use of Cold Spray Porous Coatings for Emergency Cooling of Reactor Vessels
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When a reactor vessel experiences a Loss of Coolant Accident (LOCA) or Reactivity Initiated Accident (RIA), the reactor vessel is flushed with emergency flooding to achieve rapid cooling. To achieve better safeguard performance under a catastrophic event, the Department of Energy (DoE) is interested in improving the reactor vessel’s downward facing boiling heat transfer rates under emergency flooding. To this end, interconnected, micro-porous steel coatings have shown great promise. The interconnecting channels within the porous coating provide flow paths for liquid supply and vapor escape. The additional flow paths improve durability, boiling heat transfer coefficients, and Critical Heat Flux (CHF) limits.

It is difficult to deposit porous coatings using traditional thermal spray techniques. However, Cold Spray (CS) additive manufacturing methods provide an effective solution for depositing these porous coatings. In CS, particles entrained in a heated gas stream are accelerated through a converging-diverging nozzle and undergo plastic deformation upon impact. The resulting coating is composed of randomly arranged particles and is capable of having low to high porosity levels depending upon process parameters. Preliminary studies by UJV Rez have already accomplished notable success with CS deposition of microporous coatings [1]. The current research expands upon previous work by optimizing the process and achieving three coating requirements that must be met before CS porous coatings can be mature for safeguarding applications: (1) coatings must avoid thermal mismatches and achieve desired coating porosity, (2) coatings must be able to achieve uniform deposition on complex curved surfaces, and (3) coatings must demonstrate enhanced heat transfer performance.

To achieve these criteria, the CS process parameters were systematically varied in a Design of Experiments. Optimized parameters include matrix/sacrificial materials, spray distance and velocity, carrier gas, and temperature. Once the process parameters were optimized, a coating was deposited on a hemispherical surface of a reactor vessel, as seen in Figure 1. Then, the heat transfer performance and CHF limits were tested at Penn State’s Subscale Boundary Layer Boiling (SBLB) Test Facility. Finally, thermo-mechanical testing was performed to determine bond strength and thermal cycling durability.

In conclusion, Cold Spray deposition shows great potential for improving the downward facing boiling heat transfer rates of reactor vessels under emergency cooling situations. The work may not only result in higher safety margins for catastrophic failure situations, but it may also lead to improved performance across a range of liquid handling and evaporator systems.
REFERENCES


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Modelling Intonation in Non-Western Musical Cultures
Sam Lapp, advised by Matthew Parkinson and Mark Ballora

Musical cultures across the world use tuning systems different from our twelve-tone equal temperament scale. Several mathematical models predict which notes from the Western chromatic scale are used to create harmonies and scales [1]–[4]. We find that these models cannot be extended to tuning systems used in Arabic music. We develop an alternative model in MATLAB to analyze the contextual intonation of any culture’s music. This approach avoids making assumptions about the tuning system. Initial results show interesting characteristics of intonation that distinguish Western, Arabic and Chinese music.

Methods
The model developed in this research focuses on how notes are tuned in the context of other notes. A series of consecutive notes, called a musical ‘word’, is analyzed based on the ratios of their frequencies. For instance, if three consecutive frequencies extracted from the music are 100 Hz, 150 Hz and 200 Hz, the corresponding ‘word’ is the set of ratios {1/1, 3/2, 2/1}. The MATLAB algorithm extracts frequencies from music, consolidates the frequencies into a series of distinct notes, and finds the words used. The words can contain two, three, or more consecutive notes. The set of all words used in a selection of music is called the ‘vocabulary’. By analyzing the vocabulary of a single piece, or a composer, or an entire genre, we can look for features that define them.

Initial Results
The most common intervals used in Western, Chinese and Arabic music are very distinct (Figure 1). For Western music, the most common intervals occur at the ratios in the major scale. For Chinese music, the pentatonic scale emerges. Both of these results agree with music theory. For Arabic music the results are very different. Arabic musicians use many small intervals in a highly ornamented style. The most common intervals are those close to the root (1/1).

Another interesting result is that the leading tone — the interval of the major seventh leading up a half step to the octave — is very common in Western and Arabic music, but absent in Chinese music.

Implications
This investigation has many interesting implications in designing for other cultures. First, we learn that our measurement systems may not be appropriate for describing artifacts of other cultures. For example, when analyzing Arabic music using the methods developed for Western music [1], the measurement system was insensitive to nuances that distinguish one Arabic scale from another. By forcing Arabic music to conform to a Western system of tuning, important information is lost. Next, context is important in intonation for both Western and non-Western music. Western musicians, as well as Arabic musicians, tune notes differently depending on their musical context. Traditional music notation does not capture these tuning details.

In general, Western systems of analysis and notation assume that music is played based on a fixed, discrete set of ratios inside the octave. This research challenges that view of intonation, and suggests one approach for a more flexible form of analysis. The method developed, using ‘words’ to describe a continuous pitch spectrum, may be useful for future research.
Figure 1: Most common intervals used in Western, Chinese and Arabic music

References


Art in Science
Overset Isosurfaces
Justin Kauffman, advised by Jonathan Pitt

Solution of a steady three-dimensional convection-diffusion problem with two overset meshes. The solution was obtained through a coupled overset and hybridizable discontinuous Galerkin (HDG) algorithm. Volume rendering shows the overset region. The isosurfaces provide definition for the internal structure of the three diverging sources for this solution.
Dental cement for your squid
Abdon Pena-Francesch, advised by Melik C. Demirel

SEM image of columnar epithelial cells inside the suckers of a Loligo pealei squid. These cells hold ringed teeth inside the suction cups along the arms and tentacles, which are used for prey capture.
A vector plot of velocity in a flow field, apparently showing vorticity due to improper input parameters in a particle image velocimetry cross-correlation algorithm. The algorithm calculates velocity - the vector potential of vorticity - from measured displacement fields.
Pine tree leaves like silver crystal on silicon wafer

Huihun Jung, advised by Prof. Melik Demirel

SEM image of silver particle coated silicon wafer. In the experiments of metal-assisted chemical etching (MACE), after silver particle coating on top of cleaned silicon wafer with AgNO₃, pine tree leaves like crystals were found.
The Butterfly Effect
Sema Erten, advised by Dr. Akhlesh Lakhtakia

The wing of the Chorinea Sylphina butterfly viewed through an optical microscope with 10X magnification. The red color has a pigmentary origin. Coherent scattering and diffraction from every scale’s network of parallel ridges are responsible for blue iridescence and shimmer.
An Artistic Depiction of the Laser Assisted Cold Spray Process

MICHAEL J TROWBRIDGE, ADVISED BY TIMOTHY J. EDEN

Laser Assisted Cold Spray combines the benefits of cold spray with laser heating. The heating laser follows the spray path and softens the depositing powder.
3D Bioprinted Scaffold
Kazim Kerim Moncal, advised by Ibrahim Tarik Ozbolat

Figure 1. 3D bioprinted collagen scaffold mixed with bone marrow mesenchymal stem cells (shown red) image taken using second harmonic generation microscopy by Thomas Abraham in Penn State Milton S. Hershey Medical Center.