MATERIALS
@
PURDUE

May 26th, 2023

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About

Materials @ Purdue Symposium (M@PS)

Thank you for attending Purdue's first interdisciplinary materials symposium! The Materials @ Purdue Symposium (M@PS) is a one-day event that highlights research from any material class done at Purdue. This event welcomes graduate students, post-docs, or undergraduates to present their completed or in-progress research. This symposium aims to celebrate the diversity of the field of materials within a multitude of departments at Purdue University. It also offers a platform for students to gain presentation experience, and for material researchers to learn about what other researchers are doing in our Purdue community.

Materials Engineering Graduate Student Association (MSEGSA)

The Materials Engineering Graduate School Association (MSEGSA) is a group of materials engineering graduate students dedicated to promoting and improving the academic, social and professional well-being of the graduate students in the Purdue MSE department.

If you have any questions or feedback regarding M@PS or MSEGSA events, please contact MSEGSA@purdue.edu

Useful Information

Presentations will be held at Armstrong Hall in room B061.

Breakfast will be catered from Great Harvest Bread Co, and additional **drinks** will be provided during breaks.

Lunch will be provided by Jimmy Johns, and lunchboxes will be reserved for those that have registered.

Please also note that there will be a strict **"no electronics"** policy for the duration of presentations.

The MSEGSA gratefully acknowledges funding from the College of Engineering for this event.

Timetable

MT: Metals, PO: Polymers, E: Electronics, MM: Modeling/ML, C: Composites

Presentation Itinerary

8:30–8:45	**Breakfast Catered by Great Harvest Bread Co**		
8:45–9:00	**Welcome remarks**		
9:00–9:15	MT	**Sivasubramanian Chandramouli** Michael Titus, Michael Sealy	Surface Topography Comparison Pre and Post Shot Peening on Additively Manufactured Stainless Steel and Nickel Alloy Truncheons
9:15–9:30	PO	**Geeta Pokhrel** Chelsea Davis, John Howarter	Designing Mechanically Robust Thermal Interface Materials
9:30–9:45	PO	**Akul Seshadri** Alec Lucas, Caitlin Adams, Kendra Erk, John Howarter	Superabsorbent Polymer Hydrogels in Sustainable Cement Applications
9:45–10:00	PO	**Angie Rojas Cardenas** Amy Marconnet and Chelsea Davis	Enhancing Thermal Conduction in Polymers
10:00–10:15	**Break**		
10:15–10:30	PO	**Elena Robles Molina** Nate Mosier, Junli Liu	Polyol Synthesis from Soybean Oil and High-Oleic Soybean Oil through Simplified Epoxy Ring-Opening Reactions
10:30–10:45	E	**Huilong Liu** Walter J. Smith, Isaac Berk, Kristen Tagaytayan, Edward Barnard, Thomas Beechem, Ivano Castelli, Shubhra Bansal	Bandgap Engineering of Cs-Pt Halide Perovskites by Modifying Solvent and Pt Oxidation State
10:45–11:00	E	**Bingyuan Zhao** Jordan Harriman, Aiganym Yermembetova, Alexander Wei	Radiation-Tolerant Reference Electrodes for Potentiometric Sensors in Single-Use Systems
11:00–11:15	MM	**Zhuang Mo** Guochenhao Song, Tongyang Shi, J. Stuart Bolton	Modeling of Sound Propagation in High Surface Area Granular Materials
11:15–11:30	**Break**		
11:30–1:00	**Lunch Catered by Jimmy Johns**		
1:00–1:15	MM	**Kat Nykiel** Alejandro Strachan	Semi-Supervised Prediction of Double Transition Metal MXene Stability

1:15–1:30	MM	**Md Habibur Rahman** Arun Mannodi-Kanakkithodi	Screening Defects in Semiconductors Using Graph Neural Networks
1:30–1:45	MM	**Jiaqi Yang** Arun Mannodi-Kanakkithodi	Halide Perovskite Discovery using Computational Screening and Machine Learning
1:45–2:00	MT	**Sukanya Majumder** Gyuchul Park, Daniel Murray, Mehmet Topsakal, Eric Dooryhee, Lynn Ecker, Simerjeet Gill, Maria A. Okuniewski	Microstructural Evolution of Cast and Rolled U-10wt. Percent Mo in Low Neutron Fluence Regimes at Low Temperatures
2:00–2:15	**Break**		
2:15–2:30	C	**Morgan Chamberlain** Jan-Anders Mansson	Recycling of Short Fiber Reinforced Thermoplastics in the Automotive Industry
2:30–2:45	C	**Elizabeth Montagnino** Lucy Wagner, Sam Ferengul, Thomas Siegmund, John Howarter	Nanoscale Hydration and the Micro-Structural Properties of Human Cortical Bone
2:45–3:00	C	**Sai S. Aranke** R. Byron Pipes	Platelet Critical Length for a Prepreg Platelet Molded Composite
3:00–3:15	C	**Abdullah Saad** Carlos Martinez; Rodney Trice	Development of Ablation-Resistant, High Emittance Coatings for Carbon/Carbon Composites for Hypersonic Application
3:15–3:30	**Concluding remarks**		

List of Abstracts

Oral Presentation Abstracts

Surface topography comparison pre and post shot peening on additively manufactured stainless steel and nickel alloy truncheons

Sivasubramanian Chandramouli, Michael Titus, Michael Sealy*

MT

School of Materials Engineering, *School of Mechanical Engineering

With the applications of laser powder bed fusion (L-PBF) additive manufacturing (AM) becoming omnipresent, it is important to understand and improve the mechanical and surface properties of the products to work exceptionally. The surface quality from laser powder bed fusion is typically poor due to adverse thermal management. Laser parameters, such as power, scan speed, and hatch spacing, drive melt pool dynamics and the resulting surface topography. To improve surface topography, shot peening works the surface to reduce residual peaks formed after solidification of the melt pool. The problem is that AM parts with complex geometries with intricate angles and downward facing surfaces where gravity influences the melt pool and thereby resulting in poor surface topography. The current work focuses on parts manufactured using the optimized process parameters and analyze the variation of roughness with orientation of the parts during printing and perform shot peening (SP) a prominent post-processing step for reducing the roughness (50 percent decrease in LPBF samples) and eliminating the tensile residual stress (tensile to compressive) which are formed due to the high thermal gradients. The approach was to pneumatically shot peen AM truncheons made of 316SS and IN718 with 10 different inclinations (0°- 90°) and measure areal surface features on both up-skins and down-skins. For both materials, results showed that down-skins required more peening than up-skins to achieve the same final surface topography. Thus, the research will help in understanding the surface-specific peening parameters on complex parts due to the location and orientation dependent surface roughness.

Designing mechanically robust thermal interface materials

***Geeta Pokhrel*, Chelsea Davis, John Howarter** PO

School of Materials Engineering

Thermal Interface Materials (TIMs) in electronics are typically used between heat source and heat sink to enhance heat dissipation. TIMs are exposed to harsh working conditions that can lead to failure and hinder efficient thermal conduction. Both thermal and mechanical properties are equally important for electronic reliability and performance. This study emphasizes fabricating TIMs based on polymer blend nanocomposites with mechanical robustness and sufficient thermal conductivity. The form factor of the TIM is Type II, an elastomeric/thermal pad. Prior work at Purdue fabricated pseudo-bicontinuous mechanically robust thin films of polymer blends i.e., polystyrene (PS) and polyisoprene (PI). PS and PI are glassy and rubbery polymers that respectively provide stiffness and prevent significant deformation. Imparting thermally conductive nanofillers on these robust films is our approach to function as TIMs. The thin films are fabricated through spin coating. Chemically inert gold nanoparticles were used to collect preliminary results. Later, we transitioned to 2D boron nitride (BN), an industrially relevant filler for thermal pads. This research will present initial results of morphological, mechanical, and thermal characterization of PS/PI/BN (4 vol. percent BN) nanocomposites. Transmission Electron Microscope (TEM) images show 2D BN localize at the PI phase and the interface. Both the PS/PI blend and PS/PI/BN nanocomposite were able to retain most of the original morphology on releasing from 10 percent compression. Likewise, a cross-plane conductivity value of 3.47 W/m.K was obtained for the nanocomposite. We expect the results obtained through this research will provide valuable results to scale up the processing to the industrial scale.

Superabsorbent polymer hydrogels in sustainable cement applications

***Akul Seshadri*, Alec Lucas, Caitlin Adams, Ala Douba, Kendra Erk, John Howarter** PO

School of Materials Engineering

Acrylamide-based superabsorbent polymer (SAP) hydrogels are crosslinked polymer networks capable of absorbing, holding, and releasing several times their mass in water. This behavior can be harnessed to internally cure cement by fueling the production of Calcium Silicate Hydrate (C-S-H), the main strengthening phase in concrete. C-S-H growth due to internal curing increases concrete strength and lifespan, subsequently reducing the 8 percent of global carbon emissions from cement production. Here, we aim to add a new monomer, 3-(Trimethoxysilyl) propyl methacrylate (TPM), that can polymerize into the gel network and promote heterogeneous nucleation of C-S-H and other inorganics within. This talk focuses on the polymer synthesis considerations of making Acrylamide-co-TPM gels, mainly the effect of two different solvents, water and dimethyl sulfoxide (DMSO) on the polymer structure and gel morphology. Fourier Transform Infrared Spectroscopy (FTIR) was used to analyze functionalization of the acrylamide gel with the silyl group. Discussion on the implications of the various synthesis methods and their effect on inorganic nucleation will be discussed.

Enhancing thermal conduction in polymers

Angie Rojas Cardenas**, **Amy Marconnet**, **Chelsea Davis

PO

School of Materials Engineering

Higher power densities and consumption in electronic devices require heat dissipating components with high thermal conductivity to prevent overheating and improve performance and reliability. Polymers offer advantages of low cost and weight over metallic cases, but their intrinsic thermal conductivity is low. Previous studies have shown that the thermal conduction in polymers can be enhanced by polymer chain alignment or by adding high thermal conductive fillers to create percolation paths inside the polymeric matrix. Typical thermally conductive polymers have moderate in plane conductivity, but low cross plane conductivity. Cross plane thermal conductivity is critical to removing heat from active devices and transmitting it to the external environment. In this study, we combine conductive fibers and fillers to enhance thermal conductivity of polymers without inducing significant thermal anisotropy. We fabricate our thermally conductive polymer composites by infiltrating Ultra High Molecular Weight Polyethylene (UHMW-PE) chopped fiber mats with a mixture of EGaIn liquid metal alloy and epoxy matrix. We then characterize the thermal performance of the composites using infrared thermal microscopy with two different experimental set ups that allow us to obtain values for the in plane and cross plane thermal conductivity independently. We expect that the network structure achieved by the fiber mat in combination with the liquid metal allows a uniform increase in the thermal conductivity of the composite in all directions. Future work will evaluate the mechanical performance of the composites with different stiffnesses and curing accelerant concentrations by performing cyclic loading experiments in a dynamic mechanical analyzer (DMA).

Polyol synthesis from soybean oil and high-oleic soybean oil through simplified epoxy ring-opening reactions

Elena Robles Molina, Nate Mosier, Junli Liu* PO

School of Agricultural and Biological Engineering; *University of Illinois Urbana Champaign

Plant oils allow the synthesis of novel polymer and oligomer materials, such as estolides, which can be used as lubricants. However, commercial synthesis employs expensive and hazardous catalysts such as molybdenum, meta-chloroperbenzoic acid (mCPBA), or tetrafluoroboric acid (HFB4). Here we present the optimization of epoxidation conditions for synthesizing polyols from soybean oil (SBO) and high oleic soybean oil (HOSBO) using a simplified, lower-hazard process for epoxy ring-opening reactions. Epoxides of SBO and HOSBO were formed using 30 percent hydrogen peroxide, sulfuric and acetic acids at temperatures between 30-50°C for 3-24 hrs. Epoxy-ring opening reactions were performed in a batch reaction using aqueous H2SO4 at 65°C. Epoxidation of soybean oil with this method achieved yields higher than 86.5 percent; in contrast, HOSBO achieved epoxidation yields of 94.5 percent; both results are comparable to similar commercial products. Synthesized estolides made by epoxy ring-opening reactions were evaluated in terms of hydroxyl values (HV), estolide number (EN) residual epoxy groups, GC-MS, and FTIR spectrum analysis of the disappearance of epoxy groups, and the appearance of -OH of the polyol. The resulting SBO/HOSBO polyols have HV values ranging from 165-220 mg KOH/g, and yield higher than 85 percent without stoichiometric balance to oil composition. Therefore, acid-catalyzed epoxy ring-opening reactions and low molecular weight alkyls can effectively achieve estolide synthesis. This process could enable the synthesis of tailored engine oils from low-cost renewable plant oils and higher-density polymers, thus reducing the concentration of petrochemical-based components in current fluids and wax applications.

Bandgap engineering of Cs-Pt halide perovskites by modifying solvent and Pt oxidation state

Huilong Liu, Walter J. Smith, Isaac Berk*, Kristen Tagaytayan*, Edward Barnard, Thomas Beechem**, Ivano Castelli***, Shubhra Bansal** E

School of Materials Engineering,*University of Nevada, Las Vegas,**Lawrence Berkeley National Labratory,***DTU Energy

Metal halide perovskites is an exciting materials family with excellent optoelectronic properties including broad range of visible-light absorption, tunable bandgap, high extinction coefficient, long carrier diffusion length/lifetime, and high defect tolerance. Of the wide range of perovskite compositions, APbX3 (A = Cs, MA, FA; X = I, Br, Cl) are the most explored due to promising performance for applications like photovoltaics (PV), photocatalytic devices (water splitting), X-ray detectors, light emitting diodes, etc. Due to toxicity concerns, there is an ongoing search for Pb-free halide perovskites (such as based on Sn, Ge, Bi, Sb, Cu, Ag, Ti, etc.), which can demonstrate promising optoelectronic properties as the Pb counterparts. Pt-based halide perovskites are interesting for photocatalytic devices for generation of green fuels. Here, we demonstrate the change in dimensionality and bandgap of Pt-based halide perovskites with change of Pt-oxidation state and solvent engineering.

Radiation-tolerant reference electrodes for potentiometric sensors in single-use systems

Bingyuan Zhao**, **Jordan Harriman**, **Aiganym Yermembetova**, **Alexander Wei*

E

School of Materials Engineering, *Department of Chemistry

The bioprocessing industry is gradually shifting away from stainless-steel (SS) bioreactors toward single-use (SU) systems based on thermoplastic materials. Since SU systems are disposable, they require integrated sensors that are cheap and reliable, yet can be sterilized by -irradiation for internal monitoring. Featuring simple structures and low-cost manufacturing, potentiometric sensors have great potential to be integrated into SU bioreactors. However, increased operational times and -radiation sterilization induced high energy defects present challenges to long term stability and inertness of reference electrodes (REs) of potentiometric sensing system. Here we describe thin-film REs cast on screen-printed Ag/AgCl electrodes whose inertness to changes in pH (4.5–9) and ionic strength (2–200 mM) is sufficient to support potentiometric readings with accuracies of ± 3 mV (0.05 log units) over a 60-day period. The REs are composed of polyvinyl butyral (PVB) saturated with NaCl, topped by a layer of polyurethane (PU). Exposing bilayer REs to 60Co radiation (up to 45 kGy) does not compromise inertness but introduces a voltage decay function. REs conditioned in phosphate-buffered saline (PBS, pH 7.4) at 37 celsius can achieve operational stability in less than one day and have reproducible decay functions that enable their long-term use in complex media following a single-point calibration. This was demonstrated by pairing -irradiated pH electrodes and REs to monitor pH changes in cell culture media over a 21-day period, with values within ± 0.15 pH units relative to a "ground-truth" pH meter.

Modeling of sound propagation in high surface area granular materials

Zhuang Mo, ***Guochenhao Song***, ***Tongyang Shi***, ***J. Stuart Bolton*** MM

School of Mechanical Engineering

Granular acoustical materials like activated carbon with high specific surface area owing to their meso and nano-scale porosity which enables molecular sorption effects, have drawn attention in recent research because of their excellent performance at low frequencies: for example, providing high sound absorption, and decreasing the stiffness of the mini-loudspeaker back volume. These granular materials are very different in structure from traditional acoustical treatments, such as fibrous sheets or foams. Due to their structure, the response of the granular materials exposed to incident sound waves show features that are not seen in traditional acoustic materials, and that are not predicted by models with rigid frame assumption. In our current research, a model that combines the Biot (poro-elasticity) theory and the rigid model for the high surface area granules is proposed, with the aim to address the lack of consideration of the structural wave in the latter. The model is realized with a finite difference scheme on a 2-dimensional asymmetric computational domain, representing a cross-section of a cylindrical impedance tube in which the granules are tested. This numerical approach also allows incorporation of spatially-dependent properties of the frame, and implementation of different boundary conditions. The model predictions are compared with acoustic measurements of granular materials in an impedance tube with different depths and input levels. A good match between the predictions and the measurements is obtained, validating the proposed model, and thus, providing a tool to infer the properties of such materials, and to predict their performance in noise control applications.

Semi-supervised prediction of double transition metal MXene stability

Kat Nykiel, ***Alejandro Strachan*** MM

School of Materials Engineering

MXenes are a recently-discovered class of 2D materials with important electronic, optical, and magnetic applications. Double-transition metal (DTM) MXenes are particularly of interest due to the tunability of their properties and the top-down synthesis approach of MXenes. Each DTM MXene is etched from a bulk M'M"AX phase, where each M', M", A, and X indicate a different element. This large domain of possible combinations and relative lack of synthesized examples is an excellent candidate for semi-supervised learning, where the unlabeled data is leveraged to better predict synthesizable samples. In this work, we compare several pseudo-label semi-supervised learning approaches to predict stable DTM MXenes. This was done by using previously published experimental DTM MXenes as labels and unlabeled high-throughput density-functional theory data for 8712 MAX phases. Several DTM MXenes were predicted to be stable in ambient conditions, potentially expanding the family of DTM MXenes and providing a framework for predicting synthesizability of new material candidates.

Screening defects in semiconductors using graph neural networks

Md Habibur Rahman*, *Arun Mannodi-Kanakkithodi

MM

School of Materials Engineering

Herein, we develop a framework for the prediction and screening of native defects and functional impurities in a chemical space of Group IV, III-V, and II-VI zinc blende (ZB) semiconductors. This framework is powered by crystal Graph-based Neural Networks (GNNs) trained on high-throughput density functional theory (DFT) data. Using an innovative approach of sampling dozens of metastable polymorphs from defect configurations, we generate one of the largest computational defect datasets available, containing many types of vacancies, self-interstitials, anti-site substitutions, impurity interstitials, and substitutions, as well as defect complexes. We applied three types of established GNN techniques, namely Crystal Graph Convolutional Neural Network (CGCNN), Materials Graph Network (MEGNET), and Atomistic Line Graph Neural Network (ALIGNN), to rigorously train models for predicting defect formation energy (DFE) based on a defective crystal structure as input. We find root mean square errors in DFE prediction as low as 0.2 eV, which represents a prediction accuracy of 98 percent given the range of values within the dataset, improving significantly on the state-of-the-art. Best models were applied to perform screening across thousands of hypothetical single and complex defects to find many electronically active defects which may affect the semiconductor’s performance in optoelectronic devices.

Halide perovskite discovery using computational screening and machine learning

Jiaqi Yang**, **Arun Mannodi-Kanakkithodi

MM

School of Materials Engineering

Halide perovskites are attractive materials for optoelectronic applications because of the excellent tunability of their stability and optoelectronic properties. To accelerate the exploration of promising compositions across a wide chemical space, we performed high-throughput density functional theory (DFT) computations on ABX3 halide perovskite alloys with 500 unique formulas in various cubic and non-cubic phases, using the special quasi-random structures approach for simulating mixed composition supercells. Many critical properties were computed using the semi-local GGA-PBE and hybrid non-local HSE06 functionals, including decomposition and mixing energies, electronic band gap, and spectroscopic limited maximum efficiency (SLME). We further explored polymorphism in halide perovskites by simulating larger supercell alloys with different ionic ordering and generating compounds with random octahedral distortions and rotations. This led us to a DFT dataset of 1000 compounds and their stability and optoelectronic properties, based on which we performed screening and discovered several novel materials with desirable properties. Furthermore, we applied linear correlation analysis to gain a critical understanding of how properties are influenced by specific cations and anions, their mixing fractions, the perovskite phase, and amount of strain or distortion in the lattice. We finally trained two different types of machine learning models upon the data: one using composition, structure, and level of theory information as input, and another larger model using crystal graph-based neural networks that predict properties directly from perovskite structure. These models are deployed to make predictions over thousands of hypothetical compounds, leading to the discovery of many more promising halide perovskites.

Microstructural evolution of cast and rolled U-10wt.%Mo in low neutron fluence regimes at low temperatures

Sukanya Majumder, *Gyuchul Park*, *Daniel Murray**, *Mehmet Topsakal***, *Eric Dooryhee***, *Lynn Ecker***, *Simerjeet Gill***, *Maria A. Okuniewski*

MT

School of Materials Engineering, *Idaho National Laboratories, **Brookhaven National Laboratory

Ongoing efforts to convert all high-enriched U ($>$20% U-235) -based reactors to low enriched U ($<$20% U-235) -based ones has spurred the development of U-Mo alloys as one of the most promising fuels for use in high-performance research, test, and fast reactors. As part of the qualification process, the understanding of the effects of irradiation at different temperatures and fabrication techniques on the microstructure is essential. U-10wt%.Mo fuel specimens fabricated by casting and cold rolling were irradiated in a low neutron fluence regime (0.01 and 0.1 dpa) at low temperatures (150 °C, 250 °C, and 350 °C). The microstructural evolution of the specimens was investigated using scanning electron microscopy and synchrotron X-ray diffraction. Phase decomposition of the metastable γ-U phase into the α-U and γ'-U2Mo phases was observed, with the decomposition initiating at the grain boundaries. The degree of phase decomposition increases with increasing temperature and fluence, and at 0.1 dpa and 350 °C, the entire microstructure is decomposed. A higher fraction of decomposed phases is observed in the rolled foil specimens than in the corresponding cast specimens. The grain sizes of the cast specimens (37-74 μm) are much larger than those of the foil specimens (9-15 μm), explaining the slower decomposition of the cast specimens. Since α-U exhibits much poorer irradiation behavior compared to γ-U owing to its orthorhombic structure and anisotropic nature, this decomposition is not ideal. Hence, the study demonstrates a better irradiation performance in cast U-10wt.%Mo compared to rolled.

Recycling of short fiber reinforced thermoplastics in the automotive industry

Morgan Chamberlain, *Jan-Anders Mansson*

C

School of Materials Engineering

As the demand for fiber reinforced polymer composites continues to increase alongside the need for light weighting and cost-effective design in the automotive industry, there is an increasingly pressing need for manufacturing solutions regarding the recycling and re-integration of these materials back into useful automotive applications. The following research focuses on three short fiber thermoplastic injection molding compounds relevant to the automotive industry: polypropylene (PP) reinforced with short glass fiber, polyamide-6 (PA6) with carbon fiber, and polyphthalamide (PPA) with glass and carbon fiber. This presentation will show initial results from this on-going project in collaboration with Ford Motor Company. Additionally, the project's goal will be presented in which the mechanical and thermal effects of recycling of each of these material systems are characterized; and finally, the implementation of new manufacturing solutions will be discussed that could potentially compensate for degradation in the recycled materials' properties.

Nanoscale hydration and the micro-structural properties of human cortical bone

***Elizabeth Montagnino*, Lucy Wagner, Sam Ferengul*, Thomas Siegmund*, John Howarter** C

School of Materials Engineering, *School of Mechanical Engineering

Skeletal fractures are a global issue and prevention is crucial for aging societies as risk of fracture increases with age and disease. Current therapies focusing on the biological bone remodeling cycle, help increase bone density, but reveal only a moderate impact on clinical fracture occurrence. In response, hydration at the nano structural level of bone, a composite of type I collagen and carbonated apatite, can be rethought in its role in fracture resistance and mechanical behavior. Nanoscale hydration is bound within the collagen triple helix (tightly bound), which influences the elastic modulus, and at the collagen-mineral interface (loosely bound), which mediates the load transfer between phases, both affecting the overall fracture toughness. Small-angle x-ray and wide-angle x-ray scattering (SAXS/WAXS) was used to characterize human cortical bone specimen with controlled degrees of internal hydration to investigate hydrations effect on the structural properties at the nanoscale. To modulate the water in the collagen matrix and at the collagen-mineral interface, femoral samples were partially dehydrated and demineralized in controlled environments and then treated under pharmaceutical conditions to understand the ability of the collagen to hydrate and improve the mechanical response of the bone. Experiments were complimented with finite element simulations of the residual stress states in the mineralized collagen fibril. Interface strength, and residual stress states formed from increased hydration show an affect the deformation response of cortical bone.

Platelet critical length for a prepreg platelet molded composite

***Sai S. Aranke*, R. Byron Pipes**

C

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Prepreg Platelet Molded Composites (PPMCs), consisting of an array of discontinuous unidirectional fiber-based platelets, are gaining interest due to their excellent formability. A systematic understanding of the material-structure property relation is required for their application in complex geometries. This study extends the concept of fiber critical length, which is a key marker of the fiber load transfer efficiency, to a platelet system. Unlike the simple concept of fiber critical length where fiber tensile and matrix shearing strength determine critical length, the present study utilizes damage mechanics to determine the platelet critical length. Platelet critical length is characterized as a meso-structural property, such that it cannot be viewed as a material constant where it remains strain independent. The developed computational framework evaluates effect of platelet dimensions and varying overlap morphologies on the mechanical properties of the composite utilizing a uniaxial tensile test. Cohesive zones, used to capture the interfacial interaction between platelets, identified platelet dis-bond and platelet rupture as the dominant failure mechanisms. The length of the platelet at which the failure mechanism transitions from platelet dis-bond to rupture is identified as the platelet critical length. Moreover, this study explored the sensitivity of platelet critical length to length and width overlaps, determining a critical platelet overlap ratio that maximizes system strength. This work promotes a deeper understanding of the material-structure properties of PPMCs enabling tailored platelet meso-structural arrangement for improved strength and toughness.

Development of ablation-resistant, high emittance coatings for carbon/carbon composites for hypersonic application

***Abdullah Saad*, Carlos Martinez, Rodney Trice** C

School of Materials Engineering

During re-entry, the hypersonic leading edges can experience enormous heat fluxes, with surface temperatures greater than 1600 °C expected. While carbon/carbon (C/C) is a candidate material for leading edge structures, it is prone to ablation damage above 500°C. Ablation-resistant coatings can protect the C/C, while emittance can be engineered to lower the leading-edge surface temperature through radiative cooling. Emittance is a measure of how efficiently an object emits thermal radiation compared to a perfect black body at the same temperature. Higher emittance can result in lower surface temperature by rejecting heat back to environment during aerothermal heating at re-entry phase. In this work, we have developed such ablation resistant, high emittance novel multilayer oxide coating system. The multilayer coating based on individual layers consisting of silicon carbides, zirconia, and rare-earth oxide (as emittance modifiers) is being applied to a C/C surface via pack cementation and plasma spray. Ablation tests are performed to evaluate the efficacy of the multilayer coatings in simulated high heat flux environments. We observed that the non-equilibrium tetragonal (t) ZrO2 coating stabilized Sm2O3 exhibited the best resistance to ablation, surviving 120 seconds of ablation heating without delamination from the C/C substrate. The coating significantly improved the ablation resistance of C/C by reducing the mass ablation rate of C/C by 71 percent and the linear ablation rate by 94 percent. Despite the thermal expansion mismatch, a well-defined mechanical adhesion between the substrate and the coating was observed, which may have contributed to the improved ablation resistance.