13th ANNUAL STUDENT

RESEARCH

SYMPOSIUM

April 11, 2023

Abstract Book

SOUTH DAKOTA MINES

An engineering, science and technology university

The South Dakota Mines Annual Student Research Symposium showcases research from graduate and undergraduate students across multiple disciplines on campus.

Schedule

Event Held in Surbeck Center:

Hardrock Room:

8:00 AM - 10:00 AM - Graduate Oral Sessions
10:10 AM - 12:10 PM - Graduate Oral Sessions
12:20 PM - 2:00 PM - Graduate Oral Sessions

Dorr Room:

8:00 AM - 9:40 AM - Graduate Oral Sessions
10:00 AM - 11:40 AM - Graduate Oral Sessions
12:00 PM - 1:40 PM - Graduate Oral Sessions

McKeel Room:

8:00 AM - 9:40 AM - Undergraduate Oral Sessions
9:50 AM - 11:10 AM - Undergraduate Oral Sessions
11:20 AM - 1:00 PM - Undergraduate Oral Sessions

Ballroom:

9:00 AM - 11:30 AM - Graduate Poster Session
12:01 PM - 2:30 PM - Undergraduate Poster Session

5:30 PM - 6:30 PM - Awards Ceremony

Table of Contents

Undergraduate Students

Graduate Students

Molecular Simulation of Ethanol/Water Thermodynamics in Nano-Confined Environments

Josi Stevens, Karen M. Swindler Department of Chemical & Biological Engineering
Kenneth M. Benjamin, Karen M. Swindler Department of Chemical & Biological Engineering

Separations are an important step in many chemical processes, especially in the pursuit to achieve desired purity levels in product output. A classic example of a difficult (and common) separation is that of ethanol/water. Ethanol/water mixtures are difficult to separate due to the presence of an azeotrope, which is born of strong intermolecular interactions between ethanol and water molecules in solution. Ethanol/water mixtures can be separated and purified via conventional distillation, but this requires a large amount of heat as input and one of a range of different treatments which include modulations in pressure or the addition of a third component, which add additional design and operating issues to the separation.

An alternative to conventional, energy-driven distillation, could be the use of specific materials to facilitate chemical separations. Specifically, a certain material could impart interactions between the material (wall) and the fluid as such to disrupt the network of fluid-fluid interactions that lead to azeotropes, thereby improving separation purity (and with lower energy input), for mixtures such as ethanol/water. In a much larger-scale (macroscopic) system, interactions between the fluid and the wall material have a negligible effect on the system thermodynamics. Interactions between wall material and fluid inside of a nano-confined system could have a large enough impact to influence the fluid to diverge from bulk system thermodynamic properties.

To test the above hypothesis, we have conducted grand canonical Monte Carlo simulations to probe the mixture and adsorption thermodynamics of ethanol/water mixtures in nano-confined materials (2-dimensional). The SPC/E and TraPPE force fields were used to model water and ethanol intermolecular forces, respectively, and the Steele potential was used to model the fluid-solid interactions. Specifically, the parameters of the Steele potential were systematically varied to allow characterization of materials ranging from graphene to transition metals. Simulation results include adsorption energetics and nano-confined phase diagrams, revealing the impact of nano-confinement and material type on the efficacy of chemical separation.

MOLECULAR DYNAMICS SIMULATIONS OF GRAPHENE AND GRAPHENE OXIDE: Tensile strength and Interaction with DPPC

Lan Tong, Karen M Swindler Dept. of Chemical & Biological Engineering
Sourav Verma, Karen M Swindler Dept. of Chemical & Biological Engineering Kenneth M. Benjamin, Karen M Swindler Dept. of Chemical & Biological Engineering

Graphene and its derivatives, termed graphene-family nanomaterials (GFNs), have gained considerable traction in research as novel 2D materials due to their unique physical and chemical properties. Some potential applications include biomedical device sensors, coatings to inhibit biofilm production on metal surfaces, and nanoporous filters to increase speed of desalination of seawater. Increase in production and industrial use leads to concern for occupational exposures and contribution to ambient air pollution, thus it is important to evaluate toxicity of GFNs.

The body's immune and tissue-specific responses to GFNs exposure are relatively unexplored. Inhalation is one of the main paths of the exposure; the main phospholipid in pulmonary surfactant (50% composition) is dipalmitoyl phosphatidylcholine (DPPC). It acts as a host defense and surface tension reduction. Studying the selective biomolecule such as DPPC's interaction with GFNs computationally; should aid in developing an atomistic level understanding of toxicity mechanism of GFNs.

As part of the ongoing research, Molecular Dynamics (MD) simulation was used to study the mechanical properties of graphene, and graphene oxide (GO); followed by studying the adsorption of single molecule DPPC on graphene; as a first step towards building a fundamental understanding of the interaction of GFNs with pulmonary antioxidant defense and its impact on cell functions. More specifically, the Optimized Potentials for Liquid Simulations (OPLS) and Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) force fields were used to model and simulate pristine graphene and GO, and the stress-strain curve of both 2D materials were generated. Single molecule DPPC was equilibrated near pristine graphene surface in the presence of explicit water solvent using canonical (NVT) ensemble, and its adsorption energies are reported as a function of distance from the 2D surface.

Hydrodeoxygenation of Biocrude

Zoe Fickbohm, Chemical and Biological Engineering
Rajesh Shende, Chemical and Biological Engineering

High pressure hydrodeoxygenation of untreated biocrude was studied in this work. Biocrude was generated from corn stover using hydrothermal liquefaction. Corn stover was processed in a batch reactor with high pressure and temperature. Through this process the corn stover was converted into two phases, a solid phase made of biochar, and a liquid biocrude phase. The corn stover biocrude was separated using ethanol extraction before being treated with high pressure hydrogen to create a transportation fuel substitute. The effects of hydrogen concentration, temperature, and pressure on the quality of refined biocrude were studied by changing the partial pressure of hydrogen in a nitrogen heavy environment. Both treated and untreated biocrude was analyzed using GCMS to determine the conversion of biocrude to the fuel alternative. From these results, the HHV and LHV were calculated. To be used as fuel both the HHV and LHV should be in the range of 12 kWh/kg to match diesel and gasoline specifications. These tests were compared to ASPEN plus simulations. ASPEN plus was utilized to determine the theoretical amount of hydrogen required to perform the upgrade. ASPEN plus is a chemical process simulation package that simulates the ideal scenario of a process based on user inputs. This simulation will be used in the future to determine where the inefficiencies in the system lie and allow for further optimization of the process. The results from this work will be expanded upon with the use of commercial and lab made catalysts.

Effects of Agitation Rate on Hydrolysis of Food Waste Solids in Anaerobic Digestion

Michael Hickey, Chemical and Biological Engineering
Dr. Patrick Gilcrease, Chemical and Biological Engineering

While traditional anaerobic digestion (AD) focuses on producing methane, higher value-added products may be derived from AD, including volatile fatty acids (VFAs) for biofuels. For solid organic substrates, hydrolysis is usually the rate-limiting step. Agitation likely enhances the abiotic dissolution of solid substrates but may also hinder microbial attachment needed for enzymatic hydrolysis. To investigate agitation effects on solid starch hydrolysis, batch digestions of a high starch food waster were run at five different agitation rates. Results indicate that an agitation level between the minimum suspension speed and the homogenous speed enhance hydrolysis rates. After one day, the highest agitation level (800 rpm) gave a VFA production rate 67% lower than measured at the minimum suspension speed (70 rpm); this suggests that biofilm associated hydrolysis was limited at 800 rpm. After 2 days, agitation at 25 rpm produced 29% lower VFA levels compared to 400 rpm. In separate digestion experiments using corn meal solids as the sole organic substrate, both high (400 rpm) and low agitation (135 rpm) showed separate hydrolysis benefits. Prior to 50 hours, higher agitation showed faster VFA production rates, but after 50 hours VFA production rates were faster at 135 rpm. Agitation below the just suspended speed contributes to solid layer formation and prevents abiotic dissolution. Results to date support the hypothesis that too high of an agitation rate may inhibit microbes and enzymes from interacting with food waste solids. Future research will be focused on a deeper investigation of hydrolysis where microbial attachment to solids will be quantified.

Polyhydroxyalkanoate Bioplastic for Controlled Drug Delivery

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Polyhydroxyalkanoate, or PHA, is a product of carbon storage in some bacteria. PHA can be made into bioplastic films and combined with a desired drug to create a medicinal plastic film for topical use. In this experiment, PHA was extracted from *Pseudomonas putida* by incubating the bacteria in minimal media, centrifuging out the cells and incubating in chloroform, then centrifuging the chloroform mixture and finally combining the supernatant with ethanol to precipitate out crude PHA. This crude PHA was then cast into a film by combining with acetic acid and a small amount of glycerol at a high heat. If desired, a drug and a drug linker are combined homogeneously with the mixture, and then the film was cast. Films cast with 5% and 0.5% 5-fluorouracil (a chemotherapeutic drug) and glutaraldehyde as the linker were tested on human malignant melanoma cells with a Lactate Dehydrogenase (LDH) cytotoxicity assay over time. The results showed that the 0.5% 5-FU film had maximum cytotoxicity around 48 hours of exposure to the cells, and the 5% 5-FU film had maximum cytotoxicity around 72 hours of exposure. This means that a 0.5% 5-FU film is most effective when applied for 48 hours, whereas a 5% 5-FU film would be most effective if applied for 72 hours. These initial findings provide evidence not only for the versatility of the PHA biopolymer as a drug-delivering agent, but also expand the general applications of this biopolymer.

Preparation and Applications of Hydrophobic Melamine Sponges

Audrey Dunn, Department of Chemical, Biological, and Health Sciences
Dan Heglund, Ph.D. Department of Chemical, Biological, and Health Sciences
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A Mr. Clean Magic Eraser® is useful for cleaning many surfaces because of its abrasive property and hydrophilic (water-loving) nature. The properties of the Magic Eraser can be changed to a hydrophobic (water-hating) nature when soaked in a salt solution such as $FeCl_3$ and dried. The resultant sponge now sheds water and selectively absorbs organic compounds. The hydrophilic Magic Eraser has been transformed into a hydrophobic sponge, having completely opposite properties than initially. The sponge seeks out and removes organic compounds from water and leaves the water behind, making it an excellent choice for environmental cleanup, water filtration, and even laboratory use. Recent experiments in our lab have confirmed that sponges remove nonpolar organic compounds from a water-based solution. The compound studied was trifluralin, the active ingredient of the herbicide Treflan®. It was used as a safer compound that emulates the “forever chemicals” polyfluorinated alkyl sulfonates (PFAS) that persist in environmental water and soil and negatively impact human health. Recent results in our lab show that a sponge can remove 84 percent of the trifluralin in water after 70 hours. Since the majority of the fluorinated compound was removed from the water, the sponge could be a reusable alternative to the activated carbon filtration currently used by municipal water treatment facilities. Future uses for this sponge could be to permanently remove PFAS from drinking and environmental water, soil, and testing for xenobiotic presences in food sources. Sponge preparation is simple and inexpensive, and past studies have shown regeneration and reuse after dozens of uses.

Behavior Retention in Regenerated Planaria

Lily Peterson, Logan Cole, Department of Chemistry, Biology, and Health Sciences

Dr. Kelsey Gilcrease, Department of Chemistry, Biology, and Health Sciences

Brown planaria are small, but remarkable organisms that can regenerate body tissue. Their central nervous system consists of a brain-like cerebral ganglia, nerve cords that run lengthwise down their body, and simple eyes that can sense the intensity of light. Planaria exhibit a light-evading behavioral response called negative phototaxis. Additionally, it has been found that planaria can be conditioned to stimuli like a laser light. This experiment intends to investigate the ability of the cerebral ganglia and nerve cords to retain such conditioned behavior in regenerated offspring planaria. Preliminary results showed that more frequent and intense light conditioning on the parent planaria inflicted stronger behavioral retention in the offspring planaria. During this experiment, there will be an emphasis on the difference in behavioral retention of planarian heads with regenerated tails compared to planarian tails with regenerated heads, while keeping the intensity of the light conditioning consistent for the experimental group. The results of this experiment are expected to advance the understanding of conditioned behavior in primitive organisms, which has implications for higher order organisms as well.

Bio-prospective microbes from Rapid City Water Reclamation Facility for capturing consumer derived plastics.

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Synthetic plastics have catered to the many needs of industry and daily consumption, but their durability and versatility is what makes them difficult to dispose of naturally, thus accumulating in the environment and landfills. Fortunately, microbes in the environment are equally diverse in that they manage to not only survive on numerous substrates in nature, but many can valorize those substrates and yield useful products. Over the last few years, bacterial strains have started to be discovered which can degrade commercial plastics to different extents and with different specificity. Conventionally, bacterial strains have been characterized as degraders of specific plastic types using plate assays, enzyme assays, and directly growing bacteria on plastics—often, however, the experiments are either not very selective and yield results with ambiguity, or they only consider the degradation of a single plastic type per bacteria. In this study, we evaluated eight microbial strains isolated from the Rapid City Water Reclamation Facility for their ability to grow on polypropylene (PP), polyethylene terephthalate (PET), and nitrile butadiene rubber (NBR) using numerous plate assays and by characterizing substrate degradation and signs of biofilm formation with scanning electron microscopy (SEM). To enable identification of the purity of different bacterial strains, nanopore long reads sequencing was also performed. The annotation performed on the obtained genomic sequences will offer genetic insights into the metabolic pathways involved in the process of plastic depolymerization and discuss challenges relevant to the valorization of plastic waste. The fundamental and applied knowledge generated in this project is poised to have a transformative impact on addressing the grand challenge of significantly increasing global plastic recycling in a manner that is environmentally responsible, technically feasible, economically competitive, and societally beneficial.

Keywords: Biofilms; Bioprospecting; Microbial degradation; Plastic valorization.

Review of Ontological Status of Monovalent Zinc (Zn(I)) Species – Does Zn(I) Exist?

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Peter A. Adcock, Department of Chemistry, Biology and Health Sciences

Many elementary chemistry and inorganic chemistry textbooks lead one to conclude that Zn(I) does not exist. Some twenty-first century inorganic chemistry textbooks mention the existence of Zn(I) as a diatomic species detected in fused mixtures in which the salt has been melted at a high temperature then cooled rapidly, such as $Zn/ZnCl_2$, and in organometallic compounds containing a Zn-Zn metallic bond. However, diatomic Zn(I) has left room for ambiguity about the valence of each Zn atom. Over the past two decades, some chemists have taken up the interesting challenge of synthesizing mononuclear Zn(I). Sources that have claimed to synthesize mononuclear Zn(I) using a zeolite or similar host-guest compound have reported potential for Zn(I) modified zeolites to be used as effective catalysts for reactions on methane, CO, or CO_2 to create value added products. We investigate these claims with emphasis on evidence of a unique electronic structure for Zn(I), such as paramagnetism due to an unpaired electron or reasonable spectroscopic evidence for either a $4s^2\ 3d^9$ or a $4s^1\ 3d^{10}$ electron configuration.

Sustainable Self-Watering Concrete Flowerpot

Abigail Strahl, Civil and Environmental Engineering
Heidi Sieverding, Civil and Environmental Engineering

This research focuses on creating a sustainable way to improve planters for the campus by using ceramic and glass waste while addressing weekend maintenance issues. Broken or chipped pieces of glassware or ceramics donated to secondhand stores are unsellable. Commercially manufactured self-watering planters do not have a large enough reservoir to water potted plants over the weekends during the summer on campus. In this project, the broken glass and pottery were repurposed as aggregate in concrete. The fall 2022 Civil and Environmental Engineering Freshman class created miniature planters using various additives and molds to bind the waste material. A design for a large flowerpot was developed using data collected by the Freshman. A prototype was made of the planter. The stackable pot design includes a built-in reservoir large enough for workers to leave the flowerpot unattended over the weekend. The reservoir resides at the bottom of the triangle-shaped planter. The water in the reservoir is wicked to the plants using three cotton ropes, to support plant growth and prevent wilting. A concrete mix design and casting forms were developed. With these forms, facilities and campus organizations can create as many South Dakota Mines branded planters as desired. This project upcycles ceramic and glass waste and provides facilities with a student-created design that supports campus sustainability.

Electrochemical Degradation of PFAS Chemicals

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Perfluoroalkyl and polyfluoroalkyl substances (PFASs), are a group of synthetic chemicals consisting of multiple fluorine atoms attached to an alkyl chain. These chemicals are persistent in the environment and the human body and are toxic to human health. Due to their persistence, widespread use, and unacceptable negative health effects, PFAS chemicals have been classified as an Emerging Contaminant of Concern. A variety of technologies to degrade PFASs are currently being researched and developed, but many of these methods are expensive, difficult, and highly time consuming. The research herein focuses on electrochemical destruction of PFAS chemicals. We are using an electrochemical cell called ParaCell from Gamry Instruments. The working electrode is based on thin-film Ti_4O_7 deposited on stainless steel using pulsed-laser deposition (PLD). The counter electrode is graphite and the reference electrode is Ag/AgCl. Electrolyte is 2500 ppb perfluorooctanoic acid (PFOA), 2500 ppb perfluorooctane sulfonic acid (PFOS) and 0.1 M Na_2SO_4. After running tests in the ParaCell and measuring the electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV), and open circuit voltage (OCV), we have obtained promising and reproductible results; pH is observed to drop from 5.80 to 4.57 after chronoamperometry treatment at 2.117 V against Ag/AgCl for 30 mins. This is indicative of Fenton reactions resulting in radical generation and eventual PFAS degradation. These results show that it is possible to degrade and eliminate PFAS contamination through the electrochemical method, highlighting a promising future for this technology and for the eventual reduction of PFAS chemical levels in the environment.

The Living Lab: A Geotechnical Study on Erosion

Clare Fischer, Civil and Environmental Engineering

Dr. Bret Lingwall, PhD, P.E. Civil and Environmental Engineering (Geotechnical Engineering)

When precipitation comes to Rapid City, the rain carries large volumes of sediment off of exposed soil and shale on the hills, including those surrounding the South Dakota Mines campus. A foot of sediment or more can be eroded in a single storm event causing the runoff to be black. The purpose of this study is to find cost effective solutions to retain the sediment and prevent surface erosion of the soil and shale on exposed hillsides that dot the landscape west of the Missouri River in South Dakota. Landowners, residents, and regulators need solutions that are easy to install and maintain, and low in cost. The treatment options we have explored include synthetics such as geocells, ground cover such as seed mix, and natural treatments such as wood chips and hay. So far, mechanical treatments such as erosion blankets and silt socks have proven most effective, but vegetative treatments will likely be the best option once plants are established. The main lab work of this year has been preparation for future planting and research. We have taken time to rebuild stairs and retaining walls, carve out and mulch paths, stake in silt socks to control erosion, and do general cleanup. In the spring, we will implement treatments to replace the destroyed treatments, and study the erosion that occurs using quantitative and qualitative measures. Currently, we are developing communications for the project. The lab is accessible for the public to walk around, and a website, flyers, and improved signage are being developed. This research is being done for the benefit of the citizens of Rapid City, Pennington County, and others in the region with difficult to remediate soil and shale slopes, so it is important that the results of future study are easily communicable to this audience.

Assessing the Impact of Snowfall on Traffic Accident Frequencies in Rapid City, South Dakota

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Dr. Darren Clabo, Atmospheric and Environmental Sciences, Department of Civil and Environmental Engineering

Snow events can create dangerous driving conditions. Slick roads and reduced visibility quickly deteriorate vehicle performance and driver reaction time, leading to increased vehicle crashes. Drivers accustomed to such conditions may have little concern about relatively small snow events (less than 3 inches of accumulation) that occur more frequently than major snow events (greater than 6 inches of accumulation), but this could be a false confidence. For this reason, it is possible that small snow events may have a greater effect on crash counts than major events. This study aims to quantify the relationship between car crashes and snowfall in Rapid City, an urban area of about 75,000 people in western South Dakota. It uses daily crash data from the Rapid City Police Department and daily snowfall data from the Rapid City National Weather Service Forecast Office from January 2015 to December 2019. It attempts to answer the question of how small, frequent snow events influence crash frequencies compared to large snow events. The findings of this study could be useful for emergency managers, first responders, road maintenance crews, and Rapid City drivers in general.

Temporal Tensor Factorization for Multidimensional Forecasting

Karissa Schipke (EECS), Jackson Cates (EECS)
Dr. Randy Hoover (EECS), Dr. Kyle Caudle (MATH)

In the era of big data, there is a need for forecasting high-dimensional time series that might be incomplete, sparse, and/or nonstationary. The current research aims to solve this problem for two-dimensional data through a combination of temporal matrix factorization (TMF) and low-rank tensor factorization. From this method, we propose an expansion of TMF to two-dimensional data: temporal tensor factorization (TTF). The current research aims to interpolate missing values via low-rank tensor factorization, which produces a latent space of the original multilinear time series. We then can perform forecasting in the latent space. We present experimental results of the proposed method with other state of the art methods on the Jericho-E-Usage energy dataset.

Effect of carcass size on decompositional biogeochemistry

Colette McAndrew, Department of Geology and Geological Engineering
Dr. Sarah Keenan, Department of Geology and Geological Engineering

When an animal dies, the decomposition of its carcass releases multiple compounds that become available to soil microbiota, which in turn alter soil biogeochemistry. This zone of affected substrate is known as a carcass decomposition island (CDI) and is characterized by significant changes to numerous soil characteristics including pH, conductivity, gravimetric moisture content, microbial respiration, dissolved organic carbon (DOC), and carbon (C) and nitrogen (N) stable isotopes ($\delta^{13}C$ and $\delta^{15}N$). Although differences in measurements of these parameters have been recorded for various organisms and in a variety of ecosystems, there are two notable gaps: (1) the effect of carcass size has not been investigated; and (2) prairie ecosystems are not well-studied. The present study investigates how biogeochemical parameters are affected by the decomposition of a horse carcass in a prairie ecosystem. These data were compared to those associated with the decomposition of beaver carcasses in a forest ecosystem to reveal any effects carcass size has on soil biogeochemistry. The conductivity of soils underneath the horse carcass remained elevated longer than the conductivity of soils underneath the beaver carcasses, possibly as a result of the larger carcass size. $\delta^{15}N$ values of the soil underneath the horse carcass followed similar trends to the $\delta^{15}N$ values of beaver-associated soils, exhibiting a 3.6‰ enrichment compared to control soils. However, the pH, gravimetric moisture content, and $\delta^{13}C$ values for the horse-related soil did not exhibit any trends that would indicate that the larger carcass size had a significant impact on the soil biogeochemistry. Nevertheless, this study provides the first direct comparison of the soil biogeochemistry associated with the decomposition of two different vertebrate taxa and provides more evidence of the response of certain biogeochemical parameters to carcass decomposition.

Identification of gastropod fauna for comparative paleoenvironmental reconstruction from the Beaver Creek rock shelter (39CU779), Wind Cave National Park, South Dakota

Samantha Schmidt, Geology and Geological Engineering
Dr. Nathaniel Fox, Geology and Geological Engineering

The Beaver Creek rock shelter (39CU779) is located within Wind Cave National Park, preserves the transition from the early to late Holocene from 9380±300 radiocarbon years before present (RCYBP) to 1750±60 RBYBP spanning 4.77 meters of section in the southern Black Hills of South Dakota. Many vertebrate species, terrestrial gastropods, plants, and human artifacts are preserved among the different stratigraphic layers of the site. Vertebrate taxa have been previously identified and used for paleoenvironmental reconstructions across strata. However, mollusks recovered from the site have not been identified, and the extensive number of samples collected could help construct more accurate paleoenvironmental interpretations. To fill this knowledge gap, thirty mollusk specimens were randomly sampled from levels 6 through 11. These specimens were identified to the lowest possible taxonomic level. Habitat preferences were determined for each species identified across the six stratigraphic levels based on preferences of extant members of the genus and species. The percentage of taxa that prefer discreet habitat categories were determined for each level by dividing the number of species with that habitat preference by the total species identified at each level. Gastropod faunal percentages were analyzed against vertebrate faunal percentages calculated from previous research using the same habitat types. Linear regression models were run for each preferred environment type using the percentages of species in each habitat type for each stratigraphic level to determine if there is a correlation between vertebrate and invertebrate mollusk fauna habitat preferences. These findings will help strengthen previous paleoenvironmental reconstructions of the southern Black Hills.

Analysis of the Mechanical Properties using Underground Electroformed Copper for Cryostat Tubes within the LEGEND-1000 Experiment

Abigail Sharp, Department of Materials and Metallurgical Engineering
Dr. Bharat Jasthi, Department of Materials and Metallurgical Engineering
Cabot-Ann Christofferson, Department of Chemistry, Biology, and Health Sciences

The LEGEND project has been utilizing the electroforming capabilities developed underground at the 4850 level of Sanford Underground Research Facility (SURF). The LEGEND project requires ultra-pure copper (UGEFCu) for detector parts as well as reentrant tubes that provide a division between the underground liquid argon and atmospheric argon. UGEFCu is required for this project as it has extremely low radio-contamination compared to traditional copper, generating no backgrounds in the Ge-76 detectors while possessing the mechanical and thermal properties needed in a cryogenic system that other material cannot achieve. To fabricate the reentrant tubes, the electroformed copper must be rolled and welded together multiple times. The goal of the project is to determine which process of rolling, welding, and other treatments the electroformed copper will give the desired properties needed for the LEGEND-1000 design(s).

Over the past year, various tests have been done on the copper to determine what procedures give results that meet the requirements of the reentrant tubes differing from past mechanical testing on the standard usage of UGEFCu in the MAJORANA DEMONSTRATOR experiment. Data has been collected on the UGEFCu for rolling, baseline hardness, microhardness, and tensile testing which has then been put through various steps of rolling, annealing, and welding. All samples were collected from the same piece of underground electroformed copper to provide consistency throughout the sample. This includes the weld zone, heat-affected zone, and parent material where possible. The data collected from these experiments will help design future test mock-ups and the final tube(s) for the LEGEND-1000 experiment. The current results will be discussed along with future testing.

Microstructure, Mechanical and Corrosion Properties of Tantalum Nitride and Titanium Nitride Thin Films

Avery T. Bend & Venkata A.S. Kandadai, Materials and Metallurgical Engineering
Dr. Bharat K. Jasthi, Materials and Metallurgical Engineering

The main objective of this work is to investigate the microstructure, corrosion and mechanical properties of TaN and TiN thin films deposited on Ti Substrates. Thin films of TaN and TiN were synthesized using reactive pulsed laser deposition (PLD) and reactive direct current magnetron sputtering (DCMS) techniques on Ti substrates. Two combinations of composite coatings of TaN and TiN were also synthesized by adjusting the power during the deposition process. The power used during deposition varied from 100 to 300 W for the DCMS and from 150 to 350 mJ for the PLD process. The thickness of the films was measured using in-situ ellipsometry. Raman spectral analysis and X-ray diffraction were performed to identify the phases formed in the nanocoatings. Microstructural characterization was performed using scanning electron microscopy. Preliminary analysis suggests that both TaN and TiN were successfully synthesized using reactive PLD and DCMS techniques and a positive correlation was identified between deposition power and deposition rates for both PLD and DCMS techniques.

Extreme Low Temperature Thermal Cycling on Cold Spray Deposits

Carter Crawford, Materials and Metallurgical Engineering
Dr. Grant Crawford, Materials and Metallurgical Engineering

Cold spray is a solid-state powder deposition process that is commonly used for repair applications, particularly for military components. There is an increasing need to understand how cold spray repairs perform in Earth's cold regions. The purpose of this research project is to evaluate the microstructure and mechanical stability of common aluminum cold spray deposits, often used to repair military weapon systems, when subjected to extreme low temperature thermal cycling. 6061 Al cold spray depositions were performed on Al 6061 and ZE41 Mg alloy substrates using high pressure cold spray. As-deposited specimens were subjected to thermal cycling from 25°C to −60°C for 51 cycles. Cross-sectional optical microscope and scanning electron microscope (SEM) imaging was conducted before and after thermal cycling to assess the influence of thermal cycling on the microstructure of the depositions. In addition, triple lug shear strength testing was performed to determine the adhesion strength of the cold spray depositions before and after thermal cycling. The findings from this work will provide important guidance to the U.S. Army in the implementation of 6061 Al cold spray depositions in Earth's cold regions.

Processing of Belle Fourche Shale for Use in High Strength Ceramics

Casey Mason, Department of Materials and Metallurgical Engineering
Dr. Jon J. Kellar, Department of Materials and Metallurgical Engineering

Background

A large, surface Belle Fourche Shale deposit was recently discovered on a hill adjacent to the South Dakota School of Mines campus. Upon performing X-Ray Diffraction (XRD) analysis on the mineral body, the deposit was found to be suitable for processing into a high strength ceramic material.

Mineralogy

The XRD analysis of the shale mineral body showed that there was considerable amount of montmorillonite (43 wt%). Deng and Li [1] found that montmorillonite will decompose at temperatures greater than 1000 ºC to an aluminosilicate known as mullite ($3Al_2O_3 \cdot 2SiO_2$). Mullite, as expressed by Green [2], is a favorable phase for increasing the strength of ceramic bodies. In addition, the mineral body also contains natural fluxes which will aid the vitrification process.

Processing

It was found that a moisture content of 30% was desirable for forming bricks out of the shale. To reach the desired material consistency, the mineral was added to a pug mill with the remaining 24 wt% water. The material was then mixed and extruded in the pug mill. The extruded material was then cut into bricks and fired at temperatures of 998, 1102, 1142, and 1152 ºC. The fired bricks were then sampled and XRD analysis was performed to check the mullite content.

Results

XRD showed that mullite did not begin forming until 1102 ºC. It also showed that mullite content continued to rise with increasing firing temperatures.

Conclusion

This study showed that mullite formation from Belle Fourche Shale is possible with minimal processing steps.

References

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2. Green, K. (2022) Characterization, Processing and Performance of Belle Fourche Shale for Ceramics.

Overlap Friction Stir Processing of Aluminum 6061-T6 alloys: The Impact of Overlap Percentage on Microstructure and Mechanical Properties

Author: Aaron Eastlake, Materials and Metallurgical Engineering Department
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Friction stir processing (FSP) is a solid-state processing technique used to fabricate lightweight structural materials. Overlap FSP is a two-pass technique with a certain overlap in between passes, introduced to fabricate large plates. The overlap percentage plays an important role in the microstructure evolution and mechanical properties of the processed plate. In this investigation, continuous variation in overlap percentages from -28% to 78% was performed on aluminum 6061-T6 alloy using FSP. Two variations were tested; one in which the secondary pass overlapped the advancing side of the initial pass, and another where the second pass overlapped the retreating side of the initial pass. Material flow interaction between passes exhibited substantial variation at differing overlap percentages due to pin tool offset distances. Tensile testing showed little variation in tensile properties with overlap percentage, but the weld with 50% overlap exhibited the best tensile properties. Optical microscopy of tensile samples revealed fracture locations occurring in the unprocessed regions of the advancing overlap at 50%, with fractures located in the processed region at overlap distances greater than 50%. Impact toughness with overlap on the advancing side was consistently greater than with retreating overlap, and a significant decrease in impact energy was observed when overlap exceeded 50%. Therefore, welds with 50% overlap were considered the optimal percentage for overlap FSP of aluminum 6061-T6 alloys.

Analysis of left-censored data with multiple regression techniques

Anna Hale, Department of Mathematics
Dr. Kyle Caudle, Department of Mathematics

Left-censored data is prevalent in many areas of applied scientific research, such as instrumental analysis, environmental studies, and toxicology. One main concern that arises with the attempted analysis of left-censored data is the effect on the mean within typical linear regression techniques. In this experiment, non-parametric methods including the maximum-likelihood estimate, Kaplan-Meier, and regression on order were implemented to compare estimated and true quantile values of simulated, univariate, left-censored data sets. Quantile regression methods were then applied to simulated, multivariate, left-censored data sets of various sizes and the results were evaluated based on the overall bias, median absolute errors, and root mean squared errors. Current results indicate that the Powell method in quantile regression is strongest in analyzing left-censored data. Future work includes applying expectile regression techniques on simulated data sets for comparison.

Tensor Decomposition Analysis

Brett Flerchinger, Mathematics
Dr. Kyle Caudle Mathematics
Dr. Randy Hoover, Computer Science and Engineering

RTensor2 is an R package designed to provide a common set of operations and decompositions for multidimensional arrays (tensors). It uses 6 different discrete transforms to perform its operations: discrete sine, cosine, wavelet, Walsh-Hadamard, Hartley, and the fast Fourier transforms. The purpose of this presentation is to showcase and analyze decompositions of tensors for various purposes; comparing the speed and precision of various discrete transforms used in the calculations. One application of tensors to be tested is image compression. A tensor of images has a singular value decomposition taken with a given discrete transform, then the tensors U, V, and S are truncated, making them lower rank tensors. Then, U, V, and S can be multiplied back together to generate the same set of images with only a small loss to the sharpness of the image. A second application,Linear Discriminant Analysis (LDA), is presented which: finds characteristics of different classes of images in order to identify the most probable class of a new image. LDA will be performed on images using different transforms and the accuracies will be compared.

Schlieren Imaging of Mach Diamonds

Conrad Thorman, Melissa May, & Kade Schroeder, Mechanical Engineering
Dr. Joseph John Thalakkottor, Mechanical Engineering

Mach diamonds are the arrangement of stationary waves or discs in a supersonic exhaust flow, usually from a rocket or a supersonic jet. These diamond-like shapes typically occur when the supersonic flow passes through an over-expanded nozzle and begins a cycle of contraction and expansion inside the flow boundary due to a higher atmospheric pressure. Using a double concave mirror Schlieren imaging system and the FASTCAM SA1.1/ SA1.1RV high-speed camera, we aim to observe and capture these Mach diamonds generated behind a simple water bottle rocket. In addition, this research aims to characterize the effect of varying initial conditions and nozzle shape on these Mach diamonds.

Making Spaces to Supporting Formal, Informal, and Nonformal Learning Spanning a University's Makerspace Learning Ecology

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Introduction

The purpose of this cross-case case study project [1] is to ascribe characteristics of differently oriented makerspaces across the learning ecology [2] at a singular institution. By viewing 3 specific spaces that emphasize a range of formal, informal, and nonformal learning contexts, we highlight considerations for physical, social, and cultural contexts, as well as founding design principles, metrics for success, and scalability and sustainability. With being an otherwise homogeneous corpus, this work can highlight the similarities and differences for makerspaces in educational settings.

With the introduction and ongoing incorporation of principles from the Making Community, engineering colleges have begun modifying existing project spaces and creating new makerspaces to reflect this change in mindset. However, the ongoing initiatives to reflect the more creative and less rigidly designed nature of making can be challenging to implement since many ideas are counterintuitive to existing organizational structures. This is especially true in engineering-focused entities where the parties that have historically managed existing workspaces and their resources may not be as familiar with the pedological approaches and philosophies behind these areas [3]. In addition, by the very nature of making, many common trends in makerspaces present unique challenges for the management; They require a very abstract look at the purposes and function in the settings they will operate inside.

Across One University: 3 Settings

Within a STEM-focused undergraduate school, we identify multiple workspaces available to students that provide aspects of makerspaces. The school is focused on the application of STEM learning through hands-on learning, design and project-based learning.

A. Library Makerspace as a Starting Point for All

A newly developed Library Makerspace is being installed this academic year as part of a series of initiatives in the newly renovated library space. This space is special in that it lacks a disciplinary basis and is presented as a space for all students to use, both for academic endeavors and also for fun, personal projects. It is managed and run by student life and engagement, primarily as an additional space that can provide personal and professional development for students. This space represents a new, intentionally built makerspace that has not yet developed a community of practice surrounding it.

B. Machine Shop Area for Mechanical Engineering Majors

The established traditional machine shops and 3D Printing labs that are run by the Mechanical Engineering department of the school demonstrate a classical approach to running fabrication spaces, with abundant resources available. A fistyear engineering course serves as a formal introduction to the space, with CAD and a team-based fabrication design project serving as its foundation. Safety and professional practice are an explicit set of learning goals.

C. Lab Space to Support Low- and High-Fidelity Prototying

Another space to be examined is a product design and development lab. This space is funded by the Mechanical Engineering department but is run by staff involved in the Maker Community and familiar with its concepts and approaches. This space demonstrates a classic idea of a makerspace and is the best comparison to classical makerspaces outside of higher education. Tools like a lasercutter, 3D printers, as well as low-fidelity prototyping materials are made available to student to support their course projects as well as student engineering competition teams.

Examination of Maker Values in the Designated Spaces

In these three spaces, there are many comparisons to be drawn between them, but most notably can act as microcosms of different approaches taken inside of higher education regarding the implementation of Making principles into workspaces and their learning experiences for students. Using the principles developed previously [3], a broad view analysis can be performed of each space. The machine shop and 3D Print Labs possess attributes of Practical Ingenuity [4, 5], Personal Invention, and Community Building through a peer mentorship support system. Students are encouraged to bring in their own projects, which are inspected by certain management personnel before being approved. Students then work with a mentor to produce their projects and have the opportunity eventually to work in the spaces given enough time and experience in the labs. The library, on the other hand, presents as a new, relatively undeveloped area. While the previously discussed labs have a strict hierarchy and approach to be followed, the library makerspace is a newly developed area that doesn't have a pre-existing organizational structure. In the current development life of the area, it is supposed to encourage values of Practical Ingenuity, Personal Investment, Playful Invention, Community Building, and SelfDirected Learning. However, the support of these values hasn't yet been solidified since there are still challenges in the startup of the space. Lastly, the existing lab system recently upgraded for their work. It is run by individuals who have been extensively educated on maker pedological approaches and represents the seven ideal values of a maker-based learning experience. However, the support is much more limited due to a specific focus on supporting specific classes.

Materials, Methods, and Analysis

To discuss each space in more detail and perform a qualitive analysis into how the motivations and constraints of each space effects its ability to encourage Maker-Based Learning, a systematic approach will be taken to examining each space. Each space will be researched and examined in 4 ways, to allow more direct comparisons to be drawn, and more detailed information to be available. First, a look into the organization(s) running the space will be done. Questions involving the purpose of the organization, their fiscal and educational limitations, and their perceived goal with the space will be inspected. Next, a look into the management structure of the spaces will be done. Here, the more nuanced elements of how the spaces are ran and funded will be detailed. This should give more of a practical understanding of how the spaces are truly to be ran, rather than the ideal operating conditions the owning organization operates within, can be available for a contrast between theoretical and applied support of these makerspaces. Next, the actual workspaces and resources will be inspected. How was equipment selected, how does it support the education, and how its operation effects the learning experiences will be the focus of this level of analysis. Lastly, a broader view with the previously investigated information will be taken to determine the actual motivations and limitations of the space. This large view of how the space functions as a Makerspace or lab should be invaluable to direct comparisons between the spaces.

Discussion

This leads to the discussion of results, where the individual spaces can be used to model larger contexts and situations that makerspaces in higher education may face. How does the ownership effect a makerspace? Does having fab. lab run by a specific group effect how the space grows and the culture? How does a rigid management style effect students' participation and personal investment into Making? Does a lack of definition lead to a lack of direction for a space? How does the restrictions and real-world considerations effect the culture of a space? This larger investigation should provide important context into how different factors impact a making experience.

Acknowledgement

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Adopting a Common Product Design Process Across the Undergraduate Mechanical Engineering Curriculum

Katherine Mathieu, Mechanical Engineering
Dr. Micah Lande, Mechanical Engineering

Introduction

Although most mechanical engineering undergraduate programs in the US include a capstone senior design experience, the level of training that the students receive in the product design and development process can vary considerably between programs. In some cases, students learn the product design process in parallel with their capstone senior design project. In others, there are one or more previous courses that focus on teaching different phases of the product design and development process. Also, there are other factors that impact student learning such as variations in the design process favored by each faculty member supervising a capstone senior design project, the specific design process presented and the terminology used in different product design textbooks, and the product design textbook selected for each course of a product design course sequence.

To provide students a comprehensive education in product design and development, the Mechanical Engineering Department at South Dakota School of Mines decided to implement a holistic multi-pronged strategy. First, it adopted a specific product design process as the standard reference that faculty, students, and product design related courses would consistently use. Then, it identified a design spine sequence of project courses throughout the curriculum in which the students would be exposed to different aspects related to that product design and development process. This information was codified in the department’s website and brochures where current students and prospective students could find general information about the product development process and the product design topics that students would learn in each course in the sequence.

This paper describes in detail the multi-pronged approach used in South Dakota School of Mine’s mechanical engineering undergraduate program to provide students a comprehensive education in product design and development.

The Relationship Between Material Learned in Class and Experience Gained on an Engineering Design Team

Luis Gonzalez, Mechanical Engineering
Dr. Micah Lande, Mechanical Engineering

Competing on a team like Baja or Formula on a college campus is one of the best things an engineering student can do when percussing their degree due to the range of experiences and skills gained. Most of these skills are not skills one would learn in the classroom or are not possible in the classroom setting. The freedom to experience true freedom to team, design and fail is just a few of the things that you can't do in the curriculum due to how much needs to be taught and what is being taught. To narrow down what experiences and benefits really make these types of teams special I will conduct interviews with a variety of undergrade engineering students on these teams. These interviewees will include a variety of ages as well to see if there is difference between an older team member who has had more classes in that degree work that effect experiences on their respective team. These interviews will try to find the common experiences and benefits they have gained or have had that has helped them both on there team and in the classroom, using that info we can then find a few common topics that could be weaved into the current curriculum. These common topics could help improve the current curriculum for engineers and focus in on skills that could create more rounded people and not just engineers who are great at studying and reading textbooks. If there can be a more of an emphasis on giving undergrade students more of experiences that are gained on these types of teams like working on teams and having the freedom to experiment, there should be a great improvement on creating a more well-rounded student and future engineer.

Inhibition of Macropinocytosis via Specific Inhibitors of the PI3K Pathway

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Abstract: Macropinocytosis is the process by which cells internalize large amounts of extracellular fluids, including proteins, growth factor signals, and potential surveillance of pathogens. This actin-rich process requires the activity of PI3 kinase (PI3K) to generate a signaling lipid PIP_3 for closure of macropinosomes in macrophages. However, there are other signaling lipids that are either precursors for PIP3 or are downstream products in the pathway. It is unknown to what extent these other signaling lipids play in controlling the shape and formation of macropinosomes. To further investigate the structural dynamics of macropinocytosis, the PI3K pathway must be effectively inhibited. In order to determine the extent of macropinocytosis inhibition, clathrin-mediated endocytosis (CME), the other main mechanism for uptake of material into macrophages, must also be inhibited. PI3K and CME inhibition will be optimized through a series of assays using specific inhibitors of the PI3K pathway and a known dynamin inhibitor to eliminate CME. Fluid phase uptake and CME must be inhibited independently. To differentiate between these methods of cellular uptake of materials, fluorescently tagged transferrin, a CME uptake marker, will be used to determine the effectiveness of the dynamin inhibitor at blocking CME. Once CME can be effectively inhibited, all cellular uptake will be occurring through macropinocytosis, allowing for a quantitative measurement of the inhibition of bulk fluid phase uptake via specific PI3K pathway inhibitors.

Noise Correction of Atomic Force Microscopy-Based Integrin Frequency Analysis

Logan Jundt, Nanoscience and Biomedical Engineering
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As the most common joint disorder, Osteoarthritis (OA) is problematic for countries with an aging population. In OA, the cartilage degrades which causes bone on bone contact which results in constant pain for those affected. Treatments for OA are centered around symptom relief since there is no drug approved that will slow/stop OA disease progression. The cells that make up the cartilage are called chondrocytes. These chondrocytes must regulate themselves to build and break down the cartilage when necessary through cell signaling. When this signaling isn't done properly, the chondrocytes may break down too much cartilage and result in OA. To better understand the signaling within the chondrocytes, an Atomic Force Microscope (AFM) was used to measure the movement and forces of mechanical receptor molecules (integrins) on the surface of the cell. However, because the measurements were near the sensitivity limit of the AFM, there was not enough certainty that noise (i.e., thermal, instrument and building) was not a dominant factor within the data. The focus of this project was to subtract model-based noise out of the displacement data to correct the data for further analysis. Instrument noise and building noise was found from the negative control, bare silica. Random thermal noise curves were generated based on theoretical thermal noise RMS values. A Fast Fourier Transform (FFT) was applied to each individual curve and each noise FFT was subtracted from the chondrocyte displacement curve in Python code. Inverse FFTs were applied to the resulting curves, resulting in noise-corrected time domain displacement curves. The noise-corrected curves are nearly identical to the raw data obtained from the AFM. This indicates that the data obtained from the AFM to observe the chondrocytes was likely a result of integrin movement and not thermal, building, or instrument noise.

Designing a Joint on a Chip Bioreactor: Models to Simulate Fluid Flow

Micah Hoylman, Nanoscience and Biomedical Engineering
Dr. Scott Wood, Nanoscience and Biomedical Engineering

A large part of biomedical technology research is studying diseases and their progression. Organ-on-a-chip bioreactors have emerged as a great way for researchers to observe how different cell species react in response to different induced stimuli. An *in vitro* joint-on-a-chip bioreactor was designed to analyze the progression of osteoarthritis at the cellular level. Confirmation and validation of device design is an important part of the development process of organ-on-a-chip devices. For our purposes, concentration and velocity flow were mapped in a COMSOL- Multiphysics model. This was done to validate the flow laminar flow profile through the chip as well as confirm possible degree of mixing. It was found that the velocity necessary to move cell media at a rate of 1 mL/day would not be sufficient to induce mixing inside the bioreactor.

Oxidation of Methanol to Formaldehyde in Aerobic Conditions by *Rhodobacter sphaeroides*

Whitney Ponwith, Nanoscience and Biomedical Engineering
Dr. Saurabh Dhiman, Chemistry, Biology, and Health Sciences

Methane is a potent greenhouse gas that can be oxidized by methanotrophs into useful products such as methanol and formaldehyde by utilizing the copper-dependent particulate methane monooxygenase (pMMO) enzyme. In this study, we investigated the oxidation of methanol to formaldehyde in aerobic conditions using *Rhodobacter sphaeroides* as a model organism. We grew *R. sphaeroides* in NMS media with 1% methanol as the sole source of carbon and analyzed the efficiency and conversion rate of methanol to formaldehyde and other usable C1 compounds, which are one carbon atom and its substituent(s). We used SEM and GCMS to analyze the phenotypic characteristics and microscopic variations of C1 compounds after being oxidized. Our findings provide evidence for the oxidation of methanol to formaldehyde in aerobic methanotrophs and explore the conformation of *R. sphaeroides* after being grown in a 1% methanol NMS solution. This research has implications for the optimization of methanotrophs for bioprocessing and bioremediation applications, as well as for the broader understanding of microbial metabolism and evolution.

Converting Cell Movement to Drum Beats in Python

Kat Tvrdy & Drake Van Steenwyk, Nanoscience and Biomedical Engineering

Dr. Scott Wood, Nanoscience and Biomedical Engineering

Cells are always moving and reacting to stimuli, and cartilage cells, also known as chondrocytes, are no exception. As these cells move, they can be tracked on an individual level. Using the movement of these individual cells, we intend to translate the numbers recorded on the cellular level into music, specifically different drum rhythms. This program will be used at South Dakota Mines summer camps in order to teach people how cell movement works and to help them to recognize patterns in the movement. Python is the programming language used, with Numpy, Pandas and Pygame added on in order to allow the data to be imported and read in Python. The pitch and frequency of the drum beats are based on the magnitude of the data.

A Novel Application of Power over Fiber Technology in a Photon Detection System at Cryogenic Temperatures

Alex Heindel, Physics
Diana Leon Silverio, Physics
Dr. David Martinez Caicedo, Physics

The Deep Underground Neutrino Experiment (DUNE) is an international collaboration of physicists and engineers working to design and build a next generation neutrino experiment that will help us understand more about the nature of the neutrino, which could shed light on the question of baryon asymmetry in the universe.

The DUNE experiment will work by sending a beam of neutrinos from the accelerator complex located at Fermilab in Chicago, IL to four large Liquid Argon Time Projection Chambers (LArTPCs) located a mile underground at the Sanford Underground Research Facility (SURF) in Lead, SD. One of the LArTPC will have the photon detection system embedded in the cathode. In order to have the most accurate reconstruction of neutrino events, it is imperative that the drift electric field in the LArTPC is as uniform as possible, otherwise the drift electrons will not be collected in the LArTPC wire planes making the reconstruction of the final state particles produced by the neutrino interaction difficult. One area accessed to cause fluctuations in the uniformity of the drift electric field are the copper cables used to power the photon detection system on the cathode.

To avoid using metal wires to power the DUNE photon detection system, the idea to transfer power using glass optical fibers with a high powered laser has been proposed. The optical power transferred through the fiber is then converted into electrical power using a photovoltaic power converter. While there are instances of Power over Fiber (PoF) systems being used in industry, no such application has been tried in a particle physics experiment operating at cryogenic temperatures. In this presentation, I will outline the R&D of the key components for the PoF system, and how these results will inform the future optimization of the PoF technology for the DUNE photon detection system.

The Diffusion of Radon Through Titanium for LUX-ZEPLIN

Austin Helgert, Department of Physics
Dr. Richard Schnee, Department Head and Professor of Physics

There are gaps in our knowledge and understanding of how the universe works, especially relating to the composition of dark matter, which makes up 27% of all matter and energy in the universe. To improve our understanding, the LUX-ZEPLIN (LZ) experiment uses liquid xenon to search for dark matter particles. The detection of dark matter requires a reduction of all sources of radioactivity that might be mistaken for dark matter interactions. Researchers determined that LZ's titanium cryostat emanates more radon than expected. One possible source of emanation is from diffusion, or the random movement of radon particles through the titanium. To determine if radon diffusion in titanium is higher than expected, I am measuring this diffusion by placing a high concentration of radon on one side of a titanium film and measuring the concentration of radon as a function of time on the far side of the film. I am doing this by writing code and comparing the measured results to what we expect. Computing the expected concentration requires calculating an infinite summation very precisely. If diffusion is the source for the radon in the cryostat, then the next cryostat should be constructed of a different material.

Radon Emanation Analysis of a LZ Welding Wire Sample

Kellen Weber, Department of Physics
Dr. Richard Schnee, Department of Physics

Here in South Dakota, the most sensitive dark matter detector, LUX-ZEPLIN, is spearheading the search to be the first to detect the interactions of dark matter particles with the detector's liquid xenon target. In order to detect these interactions, a 'quiet' environment is important, and the decay chain of Radon can present an issue in maintaining such an acceptable environment. In order to combat this issue, extreme caution has been taken to reduce the amount of Rn-222 that may pass into the detector's liquid xenon. Here at South Dakota Mines, we use our Radon Emanation System to find the radon decay rate of different samples sent to us. One such sample was titanium wire used to weld inside the Inner Cryostat Vessel (ICV) for the LUX-ZEPLIN experiment. I will discuss the process used to determine the rate at which radon atoms leave the Ti welding wires, including the gain correction process and what updates were necessary to better analyze the data set. I will also discuss how these results are important for finding the cause of a higher than expected emanation of radon in the titanium ICV for the LUX-ZEPLIN experiment.

Likelihood-Based Reconstruction Techniques in ANNIE

Noah Everett, Physics
Dr. Jingbo Wang, Physics

The Accelerator Neutrino Neutron Interaction Experiment (ANNIE) is a 26-ton gadolinium-doped water Cherenkov detector on the Booster Neutrino Beam at Fermilab. The primary physics goal of ANNIE is to make precision measurements of the number of final state neutrons from neutrino interactions in water to improve the systematic uncertainties of next-generation long-baseline neutrino experiments. In addition, ANNIE is also doing detector R&D on new Large Area Picosecond PhotoDetectors (LAPPDs) and Water-based Liquid Scintillator (WbLS) detector medium. To achieve ANNIE's ambitious physics goals, while fully accommodating its unique R&D campaign, a new likelihood-based reconstruction method is being developed. This reconstruction method will also allow for detailed studies of the current ANNIE detector, along with future detector configurations. In addition, the methodology used to develop this reconstruction method can be generically applied to other optical experiments for reconstruction and detector studies. The talk will first give a general overview of ANNIE and then focus on the reconstruction techniques.

Using ultra-clean conditions of the MAJORANA DEMONSTRATOR to measure unobserved ^{180m}Ta decay

Samuel Schleich, Physics
Cabot-Ann Christofferson, Chemistry, Biology, and Health Services

The decay of the nuclear isomer ^{180m}Ta has yet to be observed as it has a half-life lower limit of 8.8×10^{17} years. The conditions necessary to detect such a rare event exist only in ultra-clean, radio-silent detectors, such as the MAJORANA DEMONSTRATOR. In the current attempt to detect the ^{180m}Ta decay, 17.39 kg of high-purity Ta disks have been placed within the natural germanium detector array at the core of the MAJORANA DEMONSTRATOR, separated into different ‘string’ configurations. Here, data will be collected through October 2024.

The uniqueness of this isomer arises from the nature of its stability: the ^{180m}Ta state is more stable than its ground state, as the large spin difference between the two states suppresses a direct deexcitation. Therefore, its decay is spin-suppressed. By recording the decay of ^{180m}Ta, more accurate nuclear models can be created. At the same time, the study can be used to search for dark matter candidates that couple to the nucleus; such a coupling would cause a forced deexcitation. If this deexcitation were not to be observed, current dark matter models could be further constrained. We present an overview of the experimental setup, the installation process, and the first analysis of the data from our study—giving new half-life limits dependent on decay mode, dark matter coupling limits, and further background analysis.

This material is supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics, the Particle Astrophysics and Nuclear Physics Programs of the National Science Foundation, and the Sanford Underground Research Facility. We acknowledge the support of the U.S. Department of Energy through the LANL/LDRD Program.

Simulating Radon Movement Inside the LUX-ZEPLIN Dark Matter Detector

Tristen Olsson, Physics Department
Dr. Richard Schnee, Physics Department

One mystery at the forefront of astrophysics is dark matter. Despite comprising over 80% of all matter in the universe, it remains entirely undetected except through gravity. The goal of the LUX-ZEPLIN (LZ) experiment is to detect dark matter via a weak interaction with liquid xenon inside a Time Projection Chamber (TPC). To keep background radiation to a minimum, the experiment is located nearly a mile underground at the Sanford Underground Research Facility. However, a few prominent backgrounds remain. One such source, radon-222, can emanate into the TPC and eventually decay into lead-214, whose decay energy is similar to what we expect from a dark matter interaction. To combat these false signals, I have been developing a simulation modeling the movement of radon and its daughters in the TPC, in order to allow the positions of lead-214 decays to be predicted from other, easier to identify, decays in the radon chain. In addition to simulating motion from fluid flow, diffusion, and a uniform electric field, the project's goals include creating algorithms to infer the program's parameters from blind analysis of simulated data, creating a pairing algorithm that accurately matches decays to their parent atoms, and applying these techniques to real data from LZ itself.

Characterizing the Effects of Substrate Spiking on a Microbial Community Responsible for Caproic Acid Production

Daniel Cerfus, Chemical and Biological Engineering
Dr. Patrick Gilcrease, Chemical and Biological Engineering

Instabilities are commonly observed in anerobic digesters operating at short HRT/SRTs. A better understanding of key metabolic intermediates and their associated pathways could help explain digester community/product shifts. In this study, a semi-continuous digester was upset by an increase in agitation speed; caproic acid levels declined, and a community initially dominated by *Caproiciproducens spp.*, was subsequently dominated by *Prevotella albensis*. *Caproiciproducens spp.* utilize the reverse β-oxidation (rBOX) pathway to form medium chain fatty acids; the first step is the oxidation of an electron donor to acetyl-CoA. *Caproiciproducens spp.* will utilize both lactic acid and sucrose as electron donors in this first step. Fortuitously, *P. albensis* lacks a similar pathway and cannot utilize either substrate. If the *Caproiciproducens spp.* present in the initial consortium possesses the rBOX pathway, then spiking the digestion with lactic acid or sucrose should stimulate the production of caproic acid while minimizing the growth of *P. albensis*. Spiking the upset consortium with 5.6 g/L sucrose produced a moderate increase in caproic acid (from 0.3 to 0.8 g/L) but did not correlate with an increase in the relative abundance of *Caproiciproducens spp.*. Spiking with 5.0 g/L lactic acid resulted in a considerable jump in caproic acid (0.3 to 1.98 g/L) and corresponded to an increase in relative abundance of *Caproiciproducens spp.* and decrease of *P. albensis* (from 8 to 15% and 82 to 77%, respectively). While these results are encouraging, it is difficult to determine the direct substrate effect on individual species. As such, a pure culture, *Caproiciproducens* sp. 7D4C2, was acquired to characterize substrate effects on growth rate and VFA profiles. This pure culture was also used to screen other methods for enriching *Caproiciproducens spp.*. from an AD consortium.

Free Energy Analysis of Biomolecule Adsorption to Graphene-Cu(111) and Defective Graphene-Cu(111) Interfaces: Molecular Insights into Biofilm Formation and Adhesion

Sourav Verma, Karen M Swindler Dept. of Chemical & Biological Engineering
Dr. Kenneth M. Benjamin, Karen M Swindler Dept. of Chemical & Biological Engineering

Graphene and graphene derivatives are potential candidates to be used as biofilm inhibiting coatings for metal surfaces due to their potential antibacterial properties. Chemical vapor deposition (CVD), which involves the catalytic deposition of carbon atoms on a transition metal (such as copper), is both an alternative to mechanical exfoliation of graphite and a promising process for large scalable synthesis of graphene. However, CVD usually results in a number of structural defects and surface impurities. While defect-free graphene growth using CVD is still under investigation and these defects remain largely undesired, studies have shown defective graphene surfaces have properties distinct from the pristine layers. What remains to be known is what effect these surface defects have on biofilm adhesion and formation, since no foundational atomistic-level information is available on whether these defects produce positive or negative surface adsorption characteristics relevant to biofilm adhesion and formation.

Recent work has hypothesized that biofilm formation and adhesion may be related to the adsorption of key, early protein molecules including exopolysaccharides (EPS) to metal surfaces. Nevertheless, studies related to molecular mechanics of these early protein molecule-metal surface interaction and adsorptive performance of graphene and graphene derivative as surface coatings is rather scarce. As a first step towards exploring this hypothesis, we investigate the adsorption behaviors of 20 proteinogenic amino acids (as model compounds for microbes), the building blocks of proteins, on moire' superlattice of graphene on Cu(111), along with pristine and defect-induced graphene surfaces using molecular dynamics (MD) simulations. All the simulations were conducted in vacuum and in the presence of explicit water as solvent to deduce the effect of solvation on the adsorption behavior.

Specifically, the molecular dynamics simulations are conducted using the LAMMPS molecular dynamics simulation software package and the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) and Assisted Model Building with Energy Refinement (AMBER) potentials. The adsorption energies and the binding free energies of the amino acids on graphene-coated-Cu(111) and pristine/multi-layer/defective graphene modified surfaces are evaluated to assess the effect of surface defects on the adsorption phenomena. The adaptive biasing force technique has been used to map the complex free-energy landscapes produced by the combination of intra- and inter-molecular reaction coordinates.

Coarse-grained molecular dynamics simulation to investigate the dynamic process of adsorption of Type IV pili (T4P) (Key, early protein molecule part of the conditioning films) onto graphene and graphene-modified Copper slab (moire' superlattice Gr-Cu{111}) and its conformation change after adsorption on the surface(s), have also been studied. All the coarse-grained simulations were conducted in vacuum and in the presence of coarse-grained water as solvent to deduce the effect of solvation on the adsorption behavior.

The results of this molecular-level study should aid in developing a larger, fundamental understanding of the interaction, adsorption, and adhesion of proteins and microbes to metals and two-dimensional surfaces (with and without defects), such as found in industrial and biomedical applications.

Glass-Ceramic Phase Transformations in Sulfur-Based Electrolytes for Solid-State Lithium-Ion Batteries

Misti Acevedo, Chemistry, Biology, and Health Sciences
Dr. F. Zheng & Dr. A. White Smirnova, Chemistry, Biology, and Health Sciences

Lithium-ion batteries with an organic liquid electrolyte are known to be effective; however, they can be unsafe and difficult to safely dispose of. Because of this, there is much research into finding a suitable solid-state electrolyte. Using sulfur-based solid-state electrolytes can be a useful, sustainable, and green alternative. With their high Li^+ conductivity and transference number, electrochemical stability, and interfacial contact, sulfur-based solid-state electrolytes are ideal in lithium-ion batteries. The ionic conductivity of sulfur-based electrolytes highly depends on the crystalline phases of the products. Li_2S and P_2S_5 systems are used to form glass sulfide electrolytes which have the benefits of isotropic conduction, absence of grains, a low melting point that helps control morphology, and numerous compositions. Glass-ceramic sulfide electrolytes have the same positive traits with the addition of a superionic metastable crystalline phase although they cannot be formed by a regular solid-state reaction. This research aims to investigate the molar concentrations of Li_2S and P_2S_5 needed, using $xLi_2S\cdot(100-x)P_2S_5$ in compositions of $68 \leq x \leq 70$ mol%, to achieve the desired products. Different methods will be used for synthesis. Dry ball milling is used first, then a liquid median will be introduced in the second synthesis. This research will be using acetonitrile with the Li_2S- P_2S_5 system. Morphology of the sulfide solid electrolyte particles is obtained by using a scanning electron microscope (SEM). The crystal phase and chemical composition of the sulfide electrolytes are obtained by in-situ X-ray diffraction (XRD) and Raman spectroscopy. Electrochemical impedance spectroscopy is conducted to evaluate the ionic conductivity, and the charge rate is completed by C-rate testing. The authors acknowledge financial support from the NSF IUCRC program for supporting the “Center for solid-state electric power storage” (#2052631), and the South Dakota “Governor’s Research Center for electrochemical energy storage”.

Removal of ammonia from water using Norit Activated Carbon.

Abed Kime, Civil and Environmental Engineering
Dr. Tao Ye, Civil and Environmental Engineering

Due to the contamination of our main water sources by a vast array of pollutants, both natural and anthropogenic, the scarcity of clean water has become a global issue that impacts numerous regions across the world. One of the most common pollutants that can contaminate water sources is Ammonia.

Ammonium is a major pollutant that can significantly impact both groundwater and surface water quality. Ammonium is a form of nitrogen that can be found in various natural and anthropogenic sources, such as agricultural runoff, wastewater, and industrial discharges. It is highly soluble in water and can easily enter water sources through various pathways, such as leaching through soil and infiltration from wastewater treatment plants.

The aim of this study is to evaluate the ability of Norit activated carbon to eliminate ammonium from water, considering various parameters that can affect its effectiveness. These parameters include the pH of the water, the dosage of activated carbon, and the ammonium concentration. Batch experiments were carried out in the laboratory with different pH levels of the water and various dosages of activated carbon and ammonium concentrations. The findings demonstrate that activated carbon is highly efficient in removing ammonium from water, with a removal efficiency of up to 50%. The effectiveness of ammonium removal was found to increase with higher pH and activated carbon dosage, and lower ammonium concentration.

The Freundlich isotherm model was found to best fit the experimental data, indicating that the adsorption process is nonlinear and heterogeneous in nature. This study demonstrates the potential of activated carbon as a cost-effective and efficient method for removing ammonium from water sources. Further research is needed to investigate the performance of Norit activated carbon in treating larger volumes of water and in different water matrices.

Equilibrium and Kinetic Studies of Activated Carbon Adsorption of Iodinated X-Ray Contrast Media

Collins, Antwi Boasiako (Civil and Environmental Engineering)

Tao, Ye (PhD) (Civil and Environmental Engineering)

Iodinated X-ray contrast media (ICM) are intravenous radiocontrast agents containing iodine that are widely used for radiological visualization of human tissues and cardiovascular system in hospitals. These chemicals are poorly biodegradable and therefore cannot be effectively removed in conventional wastewater treatment plants, resulting in their presence in drinking water. ICMs can act as an iodine source in drinking water disinfection and lead to the formation of toxic iodinated disinfection byproducts. Adsorption by activated carbon presents an effective method for the removal of micro pollutants, e.g., pharmaceuticals, endocrine disrupting compounds, from wastewater and drinking water.

In this study, we investigated the removal efficiency, adsorption capacity, adsorption kinetics and effects of pH on three commercially available activated carbon for four ICM. Experimental data on ionic sodium diatrizoate showed that, Darco activated carbon provided the highest removal efficiency of 97.6%, Calgon and Norit activated carbon provided removal efficiencies of 91.49% and 89.80%, respectively. The maximum amount of adsorbate adsorbed onto Darco, Calgon, and Norit activated carbon are 277.78mg/g, 227.27mg/g and 132.75mg/g respectively. Pseudo second order kinetic model provided a better fit to the experimental data than the pseudo first oder kinetic model. The Freundlich adsorption isotherm fitted well with the experimental data for all the three activated carbons used for the studies. The effects of pH showed that, the removal efficiency of the activated carbon increases with the decrease of solution pH, with the highest removal efficiency occurring at pH 3.

Examining the Influence of Salinity on the Riparian Areas using UAS

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Salinization of soil and water is an emerging issue that influences riparian vegetation and the sustainability of water resources in the rangelands. One aspect of salinization that has been commonly observed in the sagebrush steppe and mixed grass prairie in Northwest South Dakota is rangeland degradation. Approximately 77,000 impoundments were constructed in this region by 1994 to support wildlife and livestock. Altering the hydrologic flow paths and weathering can have adverse effects on riparian corridors, surrounding landscapes, and rangeland health. The objectives of this research are: 1) to analyze and document the halophyte and halotolerant riparian plants, and 2) to determine how the riparian vegetation is correlated with the conductivity along Alkali Creek, Battle Creek, Fourmile Creek, and Antelope Creek. High-resolution UAS (unmanned aircraft systems) multispectral images will be analyzed to accomplish the objectives. The UAS sensors that record the light intensity inherent to the objects at each spatial position will be utilized for thermal imaging where the distribution of riparian vegetation along the creeks will be detected. Ortho-mosaic georeferenced DSMs (digital surface models) and 3D mapping will be developed from the aerial photographs using the software "Pix4D Mapper" to illustrate the spatial impacts of salinization in riparian vegetation. The use of UAS multispectral imaging is a reliable, cost-effective, and powerful platform for high-resolution data acquisition to examine the influence of salinization in riparian vegetation.

Nitrate Uptake Estimates throughout Diel Cycles within a Large, Oligotrophic River

Mori Staar, Civil and Environmental Engineering
Dr. Lisa Kunza, Chemistry, Biology, and Health Sciences

Excessive nitrate loading from surficial mining activity in the Elk River watershed, British Columbia has flowed into the Koocanusa Reservoir and into the Kootenai River. As loading has increased nitrogen in the river, phosphorous has remained low which may contribute to negative effects on biota in the river. Phosphorous has been added at the Idaho-Montana border annually for more than a decade to increase productivity. Nitrate uptake has been studied commonly via nutrient addition to small streams and here we focus on the nitrate depletion in a large river ecosystem and examine how it varies during the diel cycles. Our objectives are to estimate nitrate concentration, and compare trends in ecosystem metabolism between a canyon section and P addition reach, and examine how nitrate uptake varies in diel cycles. SUNA nitrate loggers along with temperature and oxygen probes will be placed in 2 locations in the river with one above the P addition at the Idaho-Montana border and one upstream of the Moyie River confluence. The average rate of nitrate uptake was 180.04 mg m^{-2} day^{-1} with a range of 0.18-494.7 mg m^{-2} day^{-1} before the P addition began, and 630.05 mg m^{-2} day^{-1} with a range of 323.14-1077.17 mg m^{-2} day^{-1} after the P addition started. Nitrate uptake and GPP appear to have a positive correlation due to both rates increasing after adding phosphorous. Before the P addition, nitrate uptake peaked at 6AM and was at its lowest 6PM. After the P addition began, the highest peak shifted to noon and lowest shifted to midnight. We concluded based on this shift that denitrification and bacteria played a larger role in nitrate uptake before the P addition and assimilation dominated after. Ecosystem metabolism increased after the P addition began, and the increased primary productivity coincided with approximately 32% increase in nitrate uptake.

Seasonal precipitation influences on water, vegetation, and soils in Northwest South Dakota

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Dr. Kurt Chowanski, Department of Chemistry, Biology, and Health Sciences

Globally, the salinization of freshwater and its interactions with surrounding soils and vegetation is becoming a more significant problem due to factors including climate change. Many of these salt-affected areas are in arid and semiarid regions of the world where water is limited and a vital resource for livestock and wildlife. Rangelands in western South Dakota are economically and ecologically affected by these phenomena through water quality, vegetation, and soil health. Regionally, water and soil salinity are influenced by weather and climate through daily, seasonal, and multi-year changes in temperature and precipitation patterns. We measured seasonal impoundment conductivity in 68 impoundments across 9 HUC12 subwatersheds from 2019 through 2022 to assess relationships with temperature, precipitation, and drought (Palmer drought severity index) data. Using multispectral satellite imagery, we evaluated whether impoundment conductivity and weather influenced vegetation and bare ground distribution surrounding the impoundments. Using classified Landsat satellite imagery to assess relationships with weather and impoundment conductivity, we buffered 100 meters from the identified impoundment edge and classified water, soil, and vegetation from 2019-2021. Overall, we saw a strong relationship where impoundment conductivity increased from the prior years' impoundment conductivity for 2019-2020 ($R^2 = 0.76$) and 2020-2021 ($R^2 = 0.54$) but not from 2021-2022 ($R^2 = 0.54$). Drought conditions and precipitation influenced seasonal impoundment conductivity relationships during the study. From 2019-2021 the classified area of open water and vegetation decreased overall, while the classified area of bare ground increased across the study area. However, in 2021-2022, the classified area of open water and vegetation increased across the study area, though not to 2019 levels. This increase in the classified area of bare ground ($r = -0.48$, $Pr < 0.001$) and decrease in classified vegetation ($r = 0.45$, $Pr < 0.001$) showed a strong relationship with annual precipitation correlated with increasing drought through 2021 and late spring and early summer precipitation in 2022. A better understanding of how changes in seasonal impoundment salinity and weather influence water quality, vegetation, and soil health will help inform decisions that could reduce the impact on livestock and wildlife in Northwest South Dakota.

Microbial Induced Corrosion Inhibition by *Citrobacter freundii* Biofilms

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Metal pipelines are prone to corrosion by highly aggressive microorganisms like sulfate-reducing *Oledesulfovibrio alaskensis* strain G20 (OA-G20). The current use of protective coatings like polymers on metals has limited efficacy with a simultaneous threat to the environment. This challenge entails the need to develop bioinspired coatings with higher corrosion resistance efficiency. Here, we studied the protective coating by biofilm matrix of *Citrobacter freundii* strain MIC21 on copper (Cu) surface to prevent Microbial Induced Corrosion (MIC). The co-culture of strain G20 and MIC21 as inocula under lactate C media exposed to the copper substrate for 60 days showed the dominance of MIC21 with no trace of G20. The passivation effect of the biofilm matrix was observed by ennoblement in open circuit potential over the corrosion test period. The formation of a compact biofilm matrix was evident from microscopy and spectroscopy that inhibited the penetration of corrosive ions into the underlying copper substrate. The pure culture of strain MIC21 and OA-G20 as controls showed corrosion inhibition by MIC21 and a high corrosion rate by OAG20 on the Cu substrate. The study provides insight into a potential application of *C. freundii* strain MIC21 biofilm for MIC prevention.

Predicting and Understanding TOX Formation Due to Chlorination/Chloramination Using Machine Learning

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Total organic halogen (TOX) is a surrogate indicator of the total halogenated disinfection by-products (DBPs), which formed during the disinfection process in water/wastewater treatment. Over 700 DBPs have been identified to date, however, currently only two groups of them are regulated by U.S. EPA. According to epidemiological studies, those regulated DBPs could not be able to fully explain the overall toxicity of DBPs. Therefore, a robust predictive model for TOX can facilitate the monitoring, analysis, and control of DBPs in water. In the study, 13 machine learning models have been developed considering influent characteristics and other experimental conditions (e.g., pH, contact time) to predict the concentration of TOX. This is the first study to apply 13 different algorithms and one chemical representation for expressing disinfectants to predict the formation of TOX. The XGBoost algorithm achieved best performance (R^2 = 0.6, RMSE, and MAE of 0.63 and 0.47, respectively) to predict TOX formation. This study addressed the use of partial dependence plots and Shapley additive explanation algorithms for in depth analysis to identify the key drivers for TOX formation. The model interpretation results indicated that properties of disinfectant, contact time, and organic content in water can significantly impact the TOX formation. Hence, the developed models have great potential to predict and understand the disinfection process in which various parameters could influence the formation of TOX.

Water Quality and Plant Community Analysis of Stock Impoundments and Rivers in a Semi-arid South Dakota Rangeland.

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Stock impoundments—otherwise known as man-made ponds—are the primary water source for livestock in the semi-arid rangelands of northwestern South Dakota. Without the presence of stock impoundments, the grazing value of these rangelands would be greatly depleted. Moreover, the water quality of these stock impoundments stands to increase or decrease grazing potential. Land managers and ranchers are tasked with providing and maintaining high quality water for livestock, and droughts and increased salinity add additional challenges. Other obstacles that are difficult to overcome include eutrophication, excess sulfates, livestock loss, and high costs associated with improving water quality. In this study, stock impoundments and four riparian areas will be assessed for changes in water quality. The stock impoundments will be split into four groups—low, medium-low, medium-high, and high. River sites will be selected to examine a range of and potential influence on the riparian vegetation. To assess water quality, samples will be obtained to examine cation and anion concentrations in the laboratory. Meanwhile in the field, electrical conductivities and pH levels of the water will be recorded. Another objective of this study is to assess how increased salinity and water quality influence riparian vegetation. To do this, plant communities will be assessed to document species richness, canopy cover, and the dominant-plant species. At the end of this study, a user-friendly guide will be developed to be able to quickly select stock impoundments with high likelihood of having good water quality.

A review of machine learning guided optical and Raman spectroscopy characterization of 2D materials

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Two-dimensional (2D) materials have gained tremendous interest in the scientific community because of their remarkable properties. Nevertheless, the dimensions of 2D materials in the nanoscale make it challenging to characterize the microstructure, evaluate the properties and identification of defects present in the materials. Traditional techniques for detecting 2D materials involved hundreds of hours of manual labor invested by researchers. Even after that, the structure-property relationships of 2D materials are perplexing and inconclusive. Machine learning (ML) deploys a wide range of algorithms to tackle the enormous datasets and extracts meaningful interpretation. ML algorithms can take the voluminous datasets as input features and streamline them to predict the fingerprint features of 2D materials within seconds. In this review, we provide the progress of ML tools in optical and Raman spectroscopy characterization of 2D materials. These two techniques are the most widely utilized tools for the initial screening of 2D materials. First, we discuss the machine-learning optical identification (MOI) method to realize the intelligent identification of 2D materials from the color characteristics of their optical micrograph. Then, we explore three algorithms: random forest regression (RFR), kernel ridge regression (KRR), and Gaussian mixture model (GMM) utilized in Raman spectroscopy to extract the valuable insights using the examples of graphene and MoS_2. Furthermore, we outline the challenges and future research prospects of ML enhanced algorithms to translate the models into industry specific applications. The fusion of ML and nanoscience provides an opportunity to accelerate the design and discovery of new 2D materials.

Advanced Two-Dimensional Protective Coatings for Pure Element Single Crystals: Corrosion Applications

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Due to its great properties such as high electrical and thermal conductivity, low surface roughness, excellent corrosion resistance, single crystalline copper (111) has gained significance attention in its application in electronics, aerospace, medical, and automotive industries. However, corrosion and degradation are some of the significant bottlenecks faced by these industries. To address these challenges, graphene incorporated advanced materials have been developed because of graphene's exceptional mechanical, electrical, and chemical properties. The graphene coated copper can address the challenges in this field by enhancing the corrosion resistance of Cu (111) and improve its performance in applications ranging from the semiconductor industry to the electronics industry. Here we have explored the effectiveness of graphene coating, a single layer (monolayer) of carbon atoms, tightly bound in a hexagonal honeycomb lattice with exceptional mechanical, electrical, and barrier properties, on Cu (111) exposed to corrosion because of the inherent barrier property of graphene. In this study, we carried out corrosion test, for 42 days, on bare {111} single-crystal copper (SC-Cu) and single-layer graphene-coated single-crystal copper (SLG/SC-Cu) and compare values such as open circuit potential, electrochemical impedance, and polarization resistance. The SLG/SC-Cu showed higher open circuit potential, higher impedance, and a lower corrosion rate compared to that of bare SC-Cu. The single-layer graphene coating acted as a barrier to corrosion and yielded lower corrosion than the bare SC-Cu. The development of corrosion-resistant advanced materials using graphene on Cu (111) holds great promise for industries facing challenges associated with degradation and corrosion. The unique properties of graphene, coupled with those of Cu (111), make it a highly attractive material for a wide range of applications in the industry. In conclusion, the development of graphene-based materials on Cu (111) has the potential to revolutionize the way we use and think about materials in industries such as semiconductors and electronics. By enhancing the corrosion resistance of Cu (111) and improving its performance, graphene-based materials offer an innovative solution to the challenges facing these industries, providing new possibilities for advanced and durable products.

Enhanced fouling and corrosion resistance of ultrathin graphene coating

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The antifouling coating industry has undergone significant upheaval as a result of the impending ban on products made with the environmentally toxic chemical tributyltin (TBT). However, fouling and corrosions are the most common threat in a wide range of industries which needs a combination of careful and costly designs to address these issues. Currently, available antifouling agents are posing serious environmental concerns due to their hazardous and toxic nature to the aquatic system. There is a real need for the continuous development of new non-toxic antifouling formulations. In that regard, a coating that has features like damage-resistant, easy to apply, hydraulically smooth, compatible with current anticorrosion coating, economical, non-toxic to non-target species, and efficient is desired. This research helps to provide an innovative antifouling strategy based on an improved understanding of the biological principles of the biofouling process with respect to sulfate-reducing bacteria. The goal of this study is to synthesize ultrathin, noninvasive graphene multilayers against microbially induced corrosion which can also act as an effective antifouling coating. In this study, graphene layers of ~100nm thickness grown on nickel substrates were evaluated for corrosion resistance performance and antifouling behavior. Based on the electrochemical investigation these coating was able to sustain the aggressive microbial attack for 30 days offering superior corrosion resistance. Optical imaging was used for the successful demonstration of the inhibition of bacterial attachment under lab conditions. The machine learning approach developed on these surfaces attested to maximum inhibition of bacterial adhesion on a coated sample which is phenomenally less than bare nickel samples. Corrosion products analyzed using various methods (XRD, Nano auger, EDS) suggested fewer corrosion products on coated samples compared to control samples. This coating strategy can be used on transition metals which play a vital role in water pipelines and the wastewater treatment sector.

An Efficient Indoor and Outdoor Localization Method Based on RSSI using Zigbee Modules

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Abstract—In many wireless sensor area networks (WSNs), finding the localization of the corresponding wireless nodes is one of the fundamental challenges. Since different types of data are transmitted among the sensor nodes, the overall communication system can only succeed if the location of each node is correctly determined for WSN applications. Moreover, with respect to wireless channel models, the received signal strength indicator (RSSI) yields a distance function. This term can thus be utilized to efficiently evaluate the distance between any two nodes. In this paper, a pair of Zigbee-based modules were used to determine the RSSI and measure the distance between them for outdoor and indoor environments. Since the Radio Frequency (RF) signal can be affected by environments, we measured the reference RSSI (dBm) at a distance of 1 meter experimentally and also evaluated the path loss exponent (α) to ensure the accuracy of the proposed technique. However, in the case of the indoor experiment, a higher error was observed compared to the outdoor environment due to the presence of physical objects as reflectors, resulting in less accuracy. The presented localization method offers a reasonable distance measurement within the range of 20 to 40 meters for outdoor and 10 to 40 meters for indoor environments.

Index terms—RSSI, Path loss exponent, WSN.

SPD Tensors: A low-dimensional discriminative data descriptor for image set classification

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In pattern recognition, the task of image set classification has often been performed by representing data using symmetric positive definite (SPD) matrices, in conjunction with the metric of the resulting Riemannian manifold. In this research, we propose a new data representation framework for image sets which we call symmetric positive definite tensor representation (SPDT). Firstly, we obtain image sets as third-order tensors, and use our SPDT model to de-scribe them. Then, we use the Riemannian kernel to map SPD tensors from the Riemannian manifold to a Hilbert space. Finally, The Support Vector Machine (SVM) classifier with the Riemannian kernel is used for image set classifica-tion. Test on three benchmark datasets shows that our SPDT model is both lower-dimensional and more discriminative data descriptor than standard SPD models for the task of image set classification. We demonstrate experimentally the superior performance of our proposed SPDT descriptors, as compared with state- of-the-art methods.

Skip-GCN: A Framework for Hierarchical Graph Representation Learning

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Dr. Randy Hoover, Electrical Engineering and Computer Science

Recently there has been high demand for the representation learning of graphs. Graphs are a complex data structure that contains both topology and features. There are several applications of graphs for social networks, such as infectious disease contact tracing and social media network communications interactions. The literature has developed methods to represent nodes in an embedding space, allowing for classical techniques to perform node classification and prediction. One such method is the graph convolutional neural network that aggregates the node neighbor's features to create the embedding. In this method, the embedding contains local information about an individual's connections but lacks the global community information about that individual. We propose a method that takes advantage of both the local and global information. We first represent information across the entire hierarchy of the network by allowing the graph convolutional network to skip neighbors in its convolutions. Then using multilinear algebra, we can capture correlations across the hierarchies to create our node embeddings by representing our convolutions as a tensor. We present experimental results for the proposed method with other state-of-the-art methods in benchmark social network datasets.

Sun Tracking Solar Power Calculation and Monitoring System Based on IoT.

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Dr. Shannon L Thornburg, Electrical Engineering and Computer Science

The internet of things is gaining popularity as more and more people learn about its advantages, and soon IoT data will be essential to our entire global civilization. With the help of the internet, we can achieve almost any goal we set our minds to. Because of the steadily rising global average temperature, more and more people are turning to alternative energy sources. One of the most common ways to get renewable energy is from the sun's rays. Technology is quickly advancing and modernizing the world. Solar energy can be used effectively and efficiently in many areas, which helps us make better use of the resources we already have. Therefore, solar power is an excellent option for our daily operations. We can save money on electricity costs if we pay attention to developing this sector and give this sector regular maintenance. But sometimes, we can not do enough physical monitoring of the solar systems because they are in places that are hard to go. With the help of the Internet of Things, we can check in on the solar energy system's current progress from any location. The main goal of this study is to improve the efficiency and reliability of solar power generation. The system uses a combination of sensors, microcontrollers, and IoT technologies to monitor solar panel performance, track the movement of the sun, and calculate the amount of solar energy generated. Due to the IoT infrastructure, we can track the solar power system's performance in real-time. The ability to monitor in real-time from anywhere is the key advantage of this technology. The system also includes a user interface that provides real-time data on solar panel performance and energy production. The proposed system has several advantages over traditional solar power systems, including higher efficiency, increased energy production, and improved reliability. The results of the study demonstrate the effectiveness of the proposed system and its potential for widespread adoption in the renewable energy industry.

Accelerated Characterization and Optimization of Thin-Film Materials with Combinatorial Deposition and Bayesian Active Learning

Terrance Life, Electrical Engineering and Computer Science
Dr. Randy Hoover, Electrical Engineering and Computer Science

Technological development is often tied to the discovery of new materials, with some periods of civilization being defined by the age's prevalent material, such as the Stone Age, Bronze Age, and Iron Age. As the pace of technical development increases, so too must the development of the materials needed to facilitate these advances. In pursuit of this, a new method is introduced which leverages combinatorial deposition and Bayesian Active Learning to perform multi-objective optimization on ternary thin-films. This method is demonstrated through the fabrication of two datasets, a pair of copper-nickel-silver alloy samples and a pair of copper-titanium-silver samples. Within these samples, the chemical composition varies by position, permitting a range of the potential sample space to be fabricated simultaneously and subsequently searched with the guidance of a Bayesian optimization algorithm using Gaussian Process models. These models were used to extrapolate the relationship between the chemical composition of the film and its surface hardness, modulus of elasticity, and electrical conductivity. From the analysis of these models, the Pareto optimal points (either minimal or maximal) between the objectives can be determined for each sample region. The single-sample models demonstrate this method's potential to simultaneously optimize multiple objectives and extrapolate the models over the entire parameter space. The subsequent multi-sample models illustrate both the potential and limitations of this framework through comparisons between the projected and true data. Finally, the suggested next steps and methods to improve the performance of the conductivity models are presented as an avenue to continue this research.

Seismic Imaging of the Southern Cascadia Subduction Zone Using a Dense Nodal Array

Lauren Stern, Geology and Geological Engineering
Dr. Kevin Ward, Geology and Geological Engineering

The Cascadia subduction zone serves as an iconic plate boundary that is known for hosting an ~ M9 megathrust earthquake with rupture patches that spanned nearly the entire length of the trench. Previous studies show that co-variation between geologic expressions at the surface and behaviors at the plate interface level, including intraslab seismicity, tremor density, plate locking, and elevated topography appear to correlate along-strike, particularly in the north at ~ 47.5°N and in the south at ~ 42.3°N. Despite there being a notable increase in these observations, there has been a lack of high resolution imaging performed in the southern forearc using modern seismic instruments. Thus, a detailed model of the structure beneath these anomalies is crucial for better understanding the seismogenic future of southern Cascadia. To image this region, we deployed a linear array of 85 three-component nodal geophones (at ~ 1 km spacing) above where the heightened geologic expressions are observed in southern Oregon during the summer of 2022 as part of the Cascadia2021 project. This newly collected dataset will fill a critical gap of imaging coverage from the surface to upper-mantle depths and will complement results gathered from previous nodal deployments to the north and south of the array. The main goals of this project are to (1) constrain the location of the plate interface, (2) characterize high and low velocity zones related to arc volcanism, and (3) determine the topography of the subducting Juan de Fuca plate.

The Use of Medical-CT to Analyze Ammonoid Shell Thickness as a Potential Response to Predation

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Dr. Sarah W. Keenan, Geology and Geological Engineering

Ammonites were members of a highly diverse subclass within *Cephalopoda* referred to as *Ammonoidea* that were very abundant and display a high degree of diversity. However, at the Jurassic-Cretaceous transition ammonoids underwent a minor extinction in which the several taxonomic families were lost. One hypothesis for extinction was an increase in the number of predators with durophagus traits, or adaptations for eating hard shelled organisms. This has been studied by examining the characteristics of hard-shelled organisms. Among other traits such as increased ornamentation, many mollusks have been observed developing thicker outer shells in the presence of durophagus predators, both within and individual's lifetime and generationally as a thicker shell becomes a selected-for trait. While this response has been observed frequently in both sedentary mollusks such as bivalves and crawling mollusks such as gastropods, it has not been examined in cephalopods. This study used medical computerized tomography (CT) to examine the average shell wall thicknesses of two ammonoid genera, *Baculites* and *Jeletzkytes*. *Baculites* are routinely preserved with evidence of predation and were expected to display a significant increase in shell wall thickness through time potentially in response to increased predation pressure. *Baculites* specimens ($n = 3$ from each time interval) show a significant increase in mean shell wall thickness ($p = 0.0137$) from the Turonian (1.1 ± 0.2 mm, mean $\pm$ standard deviation) to the Maastrichtian (2.0 ± 0.4 mm). In contrast, *Jeletzkytes* specimens did not exhibit any trends in shell wall thickness through a similar timeframe (1.0 ± 0.4 to 1.3 ± 0.5 mm). This, combined with data indicating a large increase in the diversity of several major durophagous clades during this interval, is interpreted to suggest a potential correlation between the increase in durophagous predators and the increase in shell wall thickness of *Baculites*. These results demonstrate the utility of non-destructive medical-CT analyses in fossil research.

Lithological Influences on Mosasaur Fossil Taphonomy within the Pierre Shale Formation of South Dakota

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The Pierre Shale Formation in South Dakota is divided into two geographic regions, the Black Hills Region and the Central/Eastern Region. The Missouri River divides the two geographic regions. Outcrops occurring west of the Missouri River are in the Black Hills Region and outcrops on the Missouri River Basin or east of the Missouri River are in the Central/Eastern Region. Typically, the Black Hills Region and the Central/Eastern Region have different members of the Pierre Shale outcropping. Within South Dakota, the Sharon Springs Member of the Pierre Shale also outcrops in two distinct geographic locations. Along the Missouri River, the Sharon Springs is elevated to a geologic formation. The Sharon Springs Member/Formation has mosasaur fossils present in both the Black Hills Region and the Central/Eastern Region. Given that outcrops of the Sharon Springs occur amongst different members within the two geographic regions, this study will analyze the taphonomic trends of mosasaur fossils to determine if there are significant differences in preservation trends and geochemistry. The degrees of weathering, as induced by gypsum encrustation, were tested. Additionally, X-ray fluorescence was used to determine the chemical composition of fossil specimens, specifically analyzing phosphorus, sulfur, and strontium. The mosasaur fossils do not display differences in weathering across the two geographic regions. The lack of distinct trends in weathering patterns between the Black Hills Region fossils and the Central/Eastern Region fossils is likely due to each sample set being composed of highly variable fossils. In terms of geochemistry, the fossils only display differing amounts of strontium per geographic region. The average strontium content of fossils preserved in the Black Hills Region is higher than fossils preserved in the Central/Eastern Region, with the average concentrations in parts per million being 2087.12 ppm and 1585.56 ppm respectively. The average phosphorus and sulfur contents of fossils preserved in the Black Hills Region and the Central/Eastern Region are not significantly different. Both sample sets of fossils display high variability in chemical composition. By using a regional scale, this study illustrates that specific taphonomic trends are not applicable over a large scale and variability becomes too high.

Developing a fair cost allocation using cooperative game theory with least core allocation linear programming model.

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Reduced transportation costs can be achieved through collaborative shipping, it also improves sustainability because a supply chain with fewer vehicles results in lower emissions of greenhouse gases. The least core allocation uses cooperative game theory and a sequence of linear programming models to assure fairness for all members in the grand coalition. A fair and stable allocation of common gain that maximizes savings is the least core (ensures optimal allocation) and is a solution for a fair cost allocation problem that satisfies several crucial axiomatic properties (Completeness, Rationality, and Marginality). Through a case study, we assess three companies as players collaborating within a single supply shipment as the grand coalition, using the Traveling Salesman Problem (TSP), which determines the minimal route we determine the total cost of all coalition, as they serve their customers. In this paper, we propose a model that ensures that the total cost of a trip can be fairly distributed, hence more incentive to collaborate. The proposed allocation ensures maximum savings are possible for each player as the least satisfied coalition (subgroup) is always satisfied, given that it has the propensity to disrupt the grand coalition. As a special case, we take into consideration the allocation of carbon emissions. The incentive comes from an equitable cost distribution achieved by optimizing savings for all players. With the greatest possible savings and decreased emissions as additional incentives for collaboration, this ensures both economic and environmental sustainability. To further demonstrate how well our suggested approach compares, a lexicographic comparison of allocation is made between the Shapley value and a proportionality allocation with the least core.

Friction stir processing of additively manufactured cold sprayed aluminum.

Trevor Bormann, Materials and Metallurgical Engineering
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Cold spray is a solid state coating deposition technology and has shown great promise as a new additive manufacturing method. Friction stir processing has been used as a method of improving the mechanical properties of the additve cold spray, but little analysis has been performed on the microstructural consequenses of this. In the present study, two specimens were manufactured via three iterations of cold spray and friction stir processing and were used to characterize the mixing behaviour and the microstructural effects of friction stir processing on cold spray. The first had ceramic tracers embedded in the cold spray to track the mixing characteristics and the second was homogenous 5056 aluminum used to characterize the microstructural developments. These samples were analyzed using SEM, EBSD, and EDS to characterize the mixing and microstructural developments from the process.

Recycling Enriched Germanium from an Etchant Solution

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Over the decades, many nuclear physics searches are trying to prove the hypothesis that the neutrino is its own anti-particle, proving that the lepton number is not conserved. To prove this hypothesis, the LEGEND 1000 experiment will be built entirely with enriched germanium (^{76}Ge), a slightly radioactive metalloid, as the source and detector of this rare decay event.

Since this physics event is so extremely rare, it is necessary to mitigate radioactive backgrounds that could mask the signal of neutrinoless double beta decay (0vββ). Germanium is enriched to a purity of 92% of the 76Ge isotope to generate the signal needed. This isotope can generate the 0vββ with low contamination backgrounds resulting in a more favorable signal-to-background ratio.

Multiple losses are expected during the 76Ge detector fabrication: cuttings and grindings with lubricant/water, Li or Al contacts from recycled detectors, metal with low purity, and loss during the etchant solution. To this last loss, there is not yet a developed process to recover the ^{76}Ge, which has an economic potential to save up to $5.5 million for the LEGEND 1000 project, and this is the focus of this research.

During the past year, two experimental setups were tested as well as many different recycling routes for the ^{76}Ge. These results show improvements in the recovered yield. We maintained an average of 6.5% of the fed Ge in the solid phase which can be easily recovered using a well-known wet chemistry process. This already represents approximately $357,500 in recovery. This shows how this research is promising for this objective and could be expanded for recycling other rare metals used in semiconductors.

Electric Field Enhanced Extraction of Transition Metals from NMC532 using Rotating Disc Cyclic Voltammetry in Dilute Chloride Solution

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Dr. Brett Carlson, Materials and Metallurgical Engineering

Abstract: The rising application of portable electric devices has led to the rapid accumulation of electronic wastes such as lithium-ion batteries. These wastes pose significant environmental threats when improperly disposed and contain valuable metals that could supplement the supply chain. Recycling methods that limit the potential for environmental damage and improve separation of transition metals are vital to the sustainability of battery based electrical storage. This study investigates if chemical oxidizing and reducing agents may be aided or replaced by the application of an alternating electric field to reduce surface metal oxides and subsequently accelerate reoxidation with a solubilizing anion. The electrolytic leaching mechanics of commercial battery cathode material (NMC532) in dilute hydrochloric acid were investigated using rotating disc cyclic voltammetry and ICP-MS. Future research will be required to determine how this effect translates to different leaching systems and its applicability to an industrial scale process.

The authors acknowledge financial support from the NSF IUCRC program for the "Center for solid-state electric power storage" (#2052631) and support from the South Dakota Board of Regents for the "Governor's Research Center (GRC) for electrochemical energy storage".

Microwave-assisted Sol-Gel Synthesis of High-Voltage Ruthenium-Doped $LiFePO_4$ Cathodes for Solid-State Lithium-ion Batteries

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Dr. Fan Zheng, Chemistry, Biology, and Health Sciences
Dr. Alevtina Smirnova, Chemistry, Biology, and Health Sciences

The demand for high voltage and high-capacity energy systems has grown due to increased use of portable electronics, electric vehicles, and grid energy storage systems. $LiFePO_4$ (LFP) shows great promise as a cathode material due to its low cost, structural stability, safety characteristics, and low environmental impact. However, LFP cathodes possess a low Li-ion diffusion coefficient and poor electrical conductivity compared to oxide-based cathodes that are used currently. To make LFP competitive with oxide-based cathodes, LFP was modified to improve its characteristics. Doping of materials is a highly effective method for improving electrochemical characteristics in LFP cathodes. Ruthenium-doping of iron sites within LFP has shown positive effects in the promotion of Li-ion diffusion, reduction in band gap energies, and improved electrical conductivity. Previous studies have shown that ruthenium-doping at 0.01 moles has an increased specific capacity of 162 mAh g^{-1}, better cycling characteristics, and reduced resistance compared to undoped LFP.[1] Ruthenium doping levels above 0.02 moles have shown a decrease in specific capacity, cycling characteristics, and an increased resistance due to the formation of ruthenium oxide that disrupts the crystal lattice of LFP. In this study, $LiFe_{1-x}Ru_xPO_4$ (x= 0.01, 0.0075, and 0.005) and pristine LFP were prepared via microwave-assisted sol-gel synthesis to explore the effects of lower levels of ruthenium-doping on LFP electrochemical characteristics. Microwave synthesis was employed for reduced sintering time, beneficial effects on microstructure, and decreased cost. Samples were characterized via scanning electron microscopy, in-situ/ex-situ X-ray diffraction, energy dispersive X-ray spectroscopy, electrochemical impedance spectroscopy, and cyclic voltammetry.

The authors acknowledge financial support from the NSF IUCRC program for the “Center for solid-state electric power storage” (#2052631) and support from the South Dakota Board of Regents for the “Governor’s Research Center (GRC) for electrochemical energy storage”.

1.) Gao, Y.; Xiong, K.; Zhang, H.; Zhu, B. Effect of RU Doping on the Properties of Lifepo4/c Cathode Materials for Lithium-Ion Batteries. *ACS Omega* **2021**, *6* (22), 14122–14129.

Influence of Boron Carbide in 6061 Friction Stir Processed Metal Matrix Composite Cold Spray

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Dr. Grant Crawford, Materials and Metallurgical Engineering

Metal matrix composites are of particular interest for lightweight armor applications due to their relative density and improved hardness. This research is an evaluation of friction stir processed cold spray 6061 Al - Boron Carbide metal matrix composites. The primary goals are to determine the influence of boron carbide content, and effect of varying shapes of friction stir pin tools on mechanical properties of the cold spray friction stir processed metal matrix composite. To accomplish this goal several depositions of 6061 and boron carbide, of different concentrations, are deposited on 6061 aluminum, prior to friction stir processing. Mechanical properties of interest are impact toughness, microhardness, tensile strength, ductility, and abrasion resistance. Work completed thus far is a mechanical characterization of three contents of boron carbide, using hardness, tensile, abrasion, and impact testing. Using the results from all the testing, the viability of the composite for use in armor applications can be determined.

Synthesis and thermal evaporation deposition of sodium oxychloride solid-state electrolyte for sodium-ion batteries

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Dr. Alevtina Smirnova, Department of Chemistry, Biology, and Health Sciences

Sodium-ion batteries have attracted significant attention by offering an alternative option to lithium-ion batteries. Solid-state sodium oxyhalides (Na 3 OX, X = Cl, Br, I) have the advantage of cost-effective synthesis from raw materials in a time-effective manner. In this study, sodium oxychloride (Na 3 OCl) antiperovskite was synthesized using a novel approach that allowed for facile synthesis outside of an argon glovebox. The ionic conductivity of Na 3 OCl pellets compressed between graphite-coated copper foil was tested in the temperature range of 160˚C and 200˚C using electrochemical impedance spectroscopy (EIS). Arrhenius plots demonstrated linear behavior in the whole temperature range with a calculated activation energy of 0.98 eV. At lower temperatures, EIS data was not available likely due to high impedance from the thickness of the electrolyte pellet, high activation energy, or slow migration of sodium ions through the Na 3 OCl structure. To decrease electrolyte thickness, we implement physical vapor deposition (PVD) thermal evaporation to coat thin films (<100 μm) of the electrolyte onto graphite-coated copper foil and sodium-based cathodes for use in symmetric cell and half-cell configurations. The melting and crystallization temperatures were determined using differential scanning calorimetry (DSC). The purity of as-synthesized sodium oxychloride and PVD-deposited layer was evaluated using X-ray diffraction (XRD). The results on chemical composition and crystal-to-glass phase transformations are produced from in-situ X-ray diffraction (XRD) spectroscopy in the temperature range from 25˚C up to the melting point of Na 3 OCl. Cross-sectional SEM images of PVD-deposited sodium oxychloride showed an even distribution of sodium, oxygen, and chlorine. However, XRD analysis of deposited layers showed that sodium oxychloride has a tendency to decompose into the precursors during deposition. This work is focused on maintaining the sodium oxychloride composition and structure during PVD thermal evaporation by optimizing the PVD deposition parameters.

The authors acknowledge financial support from the NSF IUCRC program for the “Center for solid-state electric power storage” (#2052631) and support from the South Dakota Board of Regents for the “Governor’s Research Center (GRC) for electrochemical energy storage”.

Microstructural Characterization and Tribological Evaluation of CrN and CrSiCN Coatings for Applications in Arctic Regions

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Transition metal nitride and nanocomposite coatings have the potential to improve the efficiency, service lifetime, and durability of equipment operating in the cold and dry environments found in Earth’s polar regions. Ceramic coatings are sensitive to their operating conditions, and development efforts have been focused on ambient and high temperature environments. Thus, there is a need to understand the influence of arctic conditions on the performance of these materials. To investigate the influence of coating phase content on cold environment performance, CrN and CrSiCN coatings were deposited by plasma enhanced reactive magnetron sputtering. Their structure, composition, mechanical properties, and wetting behavior was determined. The tribological performance of the coatings under ambient, simulated arctic, and icing conditions was evaluated with a ball-on-flat tribometer equipped with an active cooling stage and a dry compressed air source. The processing-structure-properties relationships of the coatings and their impact on the wear performance are discussed.

Investigate the effect of post-deposition heat treatment on mechanical, microstructural, and corrosion properties of NASA HR-1 cold spray deposits

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Dr. Bharat K Jasthi, Materials and Metallurgical Engineering

The main objective of this work was to investigate the microstructural, mechanical, and corrosion properties of the HR-1 (Fe-Ni superalloy) cold spray deposits as a function of spray parameters and post-deposition heat treatment temperatures. Cold spray is a solid-state deposition technique that accelerates the fine powder particles using an inert gas (He &N_2) at supersonic speeds, which plastically deforms the particles and forms a strong bond with the substrate. Microstructural characterization was performed using optical and scanning electron microscopy. Preliminary results suggest that the deposits produced with He resulted in higher microhardness and lower percent porosity. Post-deposition heat treatment was performed with the objective of improving the mechanical properties of the deposits. Electrochemical studies were performed in 3.5 wt.% NaCl solution and the corrosion potentials and corrosion rates were compared in as-deposited and post-deposition heat-treated conditions.

Keywords: HR-1, Cold spray, process gas, superalloy

Mapping skill recognition and development of undergraduate mechanical engineering students for the automotive industry

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Many undergraduate students aspiring to work in the automotive industry will pursue engineering degrees in mechanical engineering to help them attain the knowledge and skills required to compete for a position. This research project explores how undergraduate mechanical engineering students develop an understanding of how their coursework and extracurricular activities give preparation for a career trajectory in the automotive industry. Freshmen enrolled in the undergraduate mechanical engineering degree are required to complete an Introduction to Mechanical Engineering course, ME110. The course is designed to be an introduction to the mechanical engineering profession and overviews engineering fundamentals, CAD basics, professional development, and other related skills. An initial assignment these freshmen complete in this class is to imagine their future career and the steps that they will need to take to achieve it by way of finding future versions of their possible selves through the LinkedIn website. Of the 127 freshmen who completed this assignment, 25% of them aspired to work at a company that self-identifies as Motor Vehicle Manufacturing on LinkedIn. Students who are interested in a future career in the automotive industry are warned that it is a competitive space and are told to stand out with good grades and extracurricular activities that demonstrate their interest and commitment to the field. However, in a self-reported survey of the last 5 years of mechanical engineering graduates at our school (count 383), only 3% of graduates reported their first job as a company that self-identifies as Motor Vehicle Manufacturing on LinkedIn. While some students originally interested in the automotive industry may seek new passions, switch majors, pursue a master’s degree, or leave college, it appears that students may not be set up for success in their desired career path. The study examines the recognition, development, and reflection of skills for mechanical engineers in the automotive industry through qualitative, semi-structured critical incident interviews of undergraduate mechanical engineering students (n=2), recent mechanical engineering graduates from our school who successfully obtained a career in the automotive industry, and technical professional and hiring managers with much experience in the automotive industry. The insights from this research will better inform how careers in mechanical engineering may be presented to 1st-year students and how career planning might be better positioned for future engineers.

Investigation into the thermodynamic and hydrodynamics parameters of a system during Cavitation Using LAMMPS Molecular Dynamics Simulator

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Dr Joseph J. Thalakkottor. Department of Mechanical Engineering

The phenomenon of cavitation, which involves the rapid collapse of a bubble in a liquid-generating shockwave has led to damage to engineering machinery and cyclic stress on metals due to the rapid implosion of the bubbles. It has also played a major role in the medical treatment of tissues and organs. This research investigates and determines the thermodynamic and hydrodynamics parameters within and outside the bubble during the initiation and collapse phases at the molecular length scales and femtoseconds time scales. This research replicates the exact system and cavitation processes in various mediums using molecular dynamic simulations. These parameters are compared with known experimental results and analytical Rayleigh-Plesset equation to determine its accuracy and hence extrapolate this method for studying cavitation in other molecules.

Molecular dynamics simulations to verify the validity of non-linear slip in the case of TIP4P water under shear.

Hafizul Islam, Mechanical Engineering Department

Dr. Joseph John Thalakkottor, Mechanical Engineering Department

It requires some assumptions about how water flows past a surface (the boundary condition) at the solid-water interface to model water flows. A boundary condition commonly known as the no-slip condition states that water elements adjacent to a surface assume its velocity. Despite its remarkable success in replicating the characteristics of many flow types, this condition can produce unusual or singular behavior when applied to spreading water on solid substrates, corner flow, etc. Various boundary conditions have been used to resolve these difficulties by allowing finite slip at liquid-solid interfaces. However, these phenomenological models cannot provide a universal perception of momentum transfer at water/solid interfaces. Here we use molecular dynamic simulations to verify the validity of non-linear relationship between slip and shear rate in the case of TIP4P water under shear.

Role of Substrate Stiffness in Type II Diabetic Fibroblast Metabolic Rates and Their Implication on Diabetic Wound Healing

Amelia Huffer, Nanoscience and Biomedical Engineering
Tugba Ozdemir, Nanoscience and Biomedical Engineering

In people living with both type I and type II diabetes, Impaired wound healing is a major concern as the formation of ulcerated wounds can drastically reduce both the effectiveness of the healing process and the quality of life of the patient. The healing of dermal wounds particularly, involves a patients fibroblasts building up a strong extracellular matrix of mostly collagen I and collagen III fibers, which the cells of diabetic patients struggle to do. Extracellular matrix stiffness, and growth substrate stiffness in general, have already been shown to have a significant effect on the growth and development of already existent cells, and in diabetic dermal fibroblasts, morphological and physiological characteristics associated with the healing process appear to be altered from their healthy state. The goal of this study is to try to find a relationship between substrate stiffness and the characteristics of these diabetic cells, and to form a preliminary link between these disease state characteristics and the stiffness of the cells' growth substrate, hopefully clearing the way for further studies to investigate this relationship and potentially find a way to utilize it in finding a way to facilitate and speed the healing process for diabetic wounds.

Developing an inside-out staining method to acquire population statistics on the phagocytosis of large targets

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Dr. Robert Anderson & Dr. Brandon Scott, Nanoscience and Biomedical Engineering Department

Phagocytosis is the process that macrophages and other phagocytes use to internalize and destroy dead cells, debris, and antibody coated targets. The dynamic reorganization of antibodies on the target cells surface impacts the efficiency of phagocytosis. The best way we have available to capture the mobility of the antibody is using our lattice light sheet microscope, but we are limited to only looking at one cell at a time using this method. In contrast, we can use fixed cell experiments to gain population statistics for phagocytosis while sacrificing the dynamic visualization. Doing so requires the development and validation of an experimental protocol that uses inside-out staining to determine whether an antibody-coated target cell has been internalized by a macrophage. The proposed order of event includes feeding macrophages with antibody-coated target cells, fixing the cells, introducing a fluorescent secondary antibody that cannot enter the macrophage due to the size, permeabilizing the macrophages with a detergent to make holes in the membrane, introducing another secondary antibody with a different fluorophore, and finally imaging the cells. It is expected that this method will allow us to clearly delineate cells that remained outside vs cells that were eaten. After validating this method, we will be able to use the population statistics to bolster the single cell dynamics experiments. The simple inside-out staining protocol will also enable other experiments that alter the mobility of the antibody.

Imaging of NIR to Visible Upconversion Luminescence from Single $NaYF_4$: Yb^{3+}:Tm^{3+} Nanoparticles

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Dr. Steve Smith, Nanoscience and Biomedical Engineering Department

We present spectroscopic imaging of single nanoparticles of sodium yttrium fluoride co-doped with ytterbium and thulium, termed upconverting nanoparticles (UCNPs), in close proximity to noble metal nanostructures. UCNPs can convert two or more incident low energy photons into a higher energy emitted photon. This has applications in bio-imaging as well as energy-conversion devices such as solar panels. Tm-doped energy transfer upconversion (ETU) $NaYF_4$: Yb^{3+}:Tm^{3+} nanoparticles are specifically useful due to their visible (450nm) and infra-red (800nm) upconversion emission, but suffer from low quantum efficiency. The UCNPs are placed on substrates consisting of random arrangements of Ag nanowires, termed nanowire composites (NWCs) and Au nano-cavity arrays (NCAs). The NWCs and NCAs produce plasmonic enhancement of the upconversion luminescence (UCL), which is assessed using single particle spectroscopic imaging and statistical analysis. The statistical distributions from the experiments are compared to Finite Difference Time Domain (FDTD) calculations of the fields near the plasmonic substrate. Both wide field and confocal spectroscopic imaging of single UCNPs on and off the plasmonic substrates in combination with energy and time resolved spectroscopy are performed and the results are compared to a coupled rate equation analysis to elucidate the ETU enhancement mechanisms for these substrates. Our most recent work analyzing the polarization of the upconversion luminescence from single UCNPs will also be presented.

Quantifying antibody-dependent cell phagocytosis and trogocytosis using epifluorescence microscopy and flow cytometry

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Dr. Brandon Scott, Department of Nanoscience and Biomedical Engineering

Phagocytosis and trogocytosis are important mechanisms by which immune cells interact with and eliminate foreign pathogens or damaged cells. Phagocytosis involves the engulfment of target cells or particles by immune cells, while trogocytosis involves the removal of cell surface components from the target during cell-cell interactions.

In this study, we aim to develop a protocol to quantify phagocytosis and trogocytosis of antibody-labeled neutrophile-like cells when exposed to macrophages using epifluorescence microscopy and flow cytometry. This will be done by fluorescent dye-labeling the cells and antibodies that are internalized in the macrophages and differentiating them from the externalized neutrophile-like cells. The cell surface will be labeled with an NHS-ester dye and antibody labeled. Following the experiment, the cells will be exposed to TCEP a reductant that will quench surface exposed dyes. Then a red secondary fluorescence antibody will be used to identify cells not internalized by the macrophages. The expectation is that internalized cells will not be quenched by TCEP and remain fluorescent. Some parts of the cell will be internalized for trogocytosis and escape the dye quenching. At the same time, there may be enough primary antibodies for the red secondary fluorescent antibodies to label the externalized cells. The variations of the trogocytosis will be filled by varying the mobility of the neutrophile-like cells. This would be confirmed using flow cytometry and epifluorescence microscopy. The results of this study will assist in providing important insights into the complex interactions between immune cells and their targets and may have implications for the development of novel therapies for immune-related diseases.

Polarization and Spectrally resolved Multiphoton Fluorescence, Luminescence and Second Harmonic Imaging in Nano-Biomaterials

Tolulope Ajuwon – Nanoscience and Nanoengineering
Dr. Steve Smith - Nanoscience and Nanoengineering

We present polarization-resolved and spectrally resolved multi-photon induced fluorescence (TPIF) and second harmonic generation (SHG) imaging in nano-biomaterials including porcine arterial wall tissue sections and the single atomic layer 2D material tungsten di-selenide. The porcine arterial wall tissue comprises of both native tissues and damaged tissues subject to a proprietary therapy based on photo-activated crosslinking of collagen and other structural proteins in the arterial wall, a proposed treatment for peripheral artery disease termed non-invasive vascular scaffolding (NVS). The tungsten di-selenide samples are exfoliated monolayer flakes supported on glass substrates. We employ a spectrally resolved multi-photon imaging system, based on a closed loop piezoelectric stage, a transmission grating and an EMCCD. From the spectrally resolved multiphoton emission of the porcine arterial cross-sections, we form ratiometric images of select spectral bands associated primarily with collagen (SHG) and elastin (TPIF) to identify characteristic micro-distributions to reveal the relative elastin and collagen composition of the tissue sections and their properties before and after formation of the NVS. We also analyze the polarization dependent SHG from monolayer WSe_2 and its relation to the crystal symmetry and orientation. The angular dependence of SHG is used to confirm and distinguish single WSe_2 from staking dependent double (2H) and triple (3R) stackings of multi-layer flakes. Spatially resolved luminescence reveals the presence of edge states and localized defects.

Hyaluronic Acid Binding Peptide (HABP) Functionalized Electrospun PCL Fibers as a Candidate for Building an Artificial Synovial Membrane

Hosein Mirazi, Nanoscience and Biomedical Engineering

Dr. Scott Wood & Dr. Tugba Ozdemir, Nanoscience and Biomedical Engineering

Statement of Purpose

Synovial membranes line articular joints, and the cells that consist of them play a key role in regulating the composition of the synovial fluid of the joint. Also, the Synovial membrane is made of hyaluronic acid. Unlike most other barrier membranes found in the body, the synovial membrane lacks a basement membrane and is instead composed of a dense type IV collagen (Col4) network (ground matrix) embedded that is interspersed with cells and type I collagen (Col1) bundles. There are two primary cell types found within the synovial membrane: fibroblast-like synoviocytes (FLSs) and macrophage-like synoviocytes (MLSs). In this project, we will replicate the structure and composition of the synovial membrane using electrospun poly-ε-caprolactone (PCL) fibers functionalized with a Hyaluronic acid binding peptide (HABP) sequence. We hypothesize that HABP functionalized fibers are suitable scaffolds to induce fibroblast to deposit cartilage extracellular matrix reminiscent of synovial membranes and could be potentially good candidate for building an artificial synovial. In this project, we also have been doing some characterization like stiffness, porosity, contact angle and surface roughness.

Summary of Results:

PCL scaffolds are produced, and the fiber morphology is intact, the average fiber diameter was measured as 0.96±0.36 µm. Viability measurements between Ctrl and HABP group did not indicate statistically significant difference. Moreover, more than 90% viability was observed, with the total number of dead cells and live cells being similar for both groups.

Conclusions

HABP on these scaffolds was not found to be toxic to these cells. Further experiments will be performed as described in the methods, in which we expect to observe that using PCL fibers with HABP will initiate HA deposition and upregulate expression of other FLS markers.

Photothermal attenuation of cancer cell stemness, chemoresistance and migration using CD44 targeted MoS2 nanosheets

Jinyuan Liu, Nanoscience and Biomedical Engineering
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Cancer stem-like cells (CSCs) play key roles in chemoresistance, tumor metastasis, and clinical relapse. However, current CSC inhibitors lack specificity, efficacy, and applicability to different cancers. Herein, we introduce a nanomaterial-based approach to photothermally induce the differentiation of CSCs, termed “Photothermal Differentiation”, leading to the attenuation of cancer cell stemness, chemoresistance, and metastasis. MoS_2 nanosheets and a moderate photothermal treatment were applied to target a CSC surface receptor (i.e., CD44) and modulate its downstream signaling pathway. This treatment forces the more stem-like cancer cells to lose the mesenchymal phenotype and adopt an epithelial, less stem-like state, which shows attenuated self-renewal capacity, more response to anticancer drugs, and less invasiveness. This approach could be applicable to various cancers due to the broad availability of the CD44 biomarker. The concept of using photothermal nanomaterials to regulate specific cellular activities driving the differentiation of CSCs offers a new avenue for treating refractory cancers.

Keywords: MoS_2 nanosheets, CD44, photothermal differentiation, cancer cell stemness, chemoresistance

Inducing tumor endothelial leakiness to enhance drug delivery using CD146 targeted gold nanorods and mild hyperthermia

Xiao Yu & Jinyuan Liu, Nanoscience and Biomedical Engineering

Dr. Congzhou Wang, Nanoscience and Biomedical Engineering

The enhanced permeability and retention (EPR) effect has been utilized as a major strategy for the delivery of nano-therapeutics and anticancer drugs to tumors. However, this effect is not always reliable, as some tumors do not possess a leaky endothelium that is required for the EPR effect. In order to reduce absolute reliance on the EPR effect, inducing endothelial leakiness at the tumor site could be exploited as a potential strategy to increase the effectiveness of nanomedicine-based or conventional anticancer therapies. Gold nanorods (AuNRs) are highly biocompatible, easy to be surface-functionalized, and have the unique photothermal properties. The cluster of differentiation 146 (CD146), a cancer cell adhesion molecule, is over-expressed on the surfaces of tumor endothelial cells. When combining CD 146 targeted AuNRs with a mild hyperthermia, we hypothesize that the synergistic effects can induce a greater degree of endothelial leakiness at the tumor sites, which facilitates the delivery of nanotherapeutics and anticancer drugs to tumors.

Defining the Efficiency of Phagocytic Events using Lattice Light Sheet Microscopy

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Macrophages are innate immune cells responsible for phagocytosis, to maintain homeostasis in organisms by clearing pathogens, debris, and apoptotic cells. Phagocytosis is initiated by receptor complexes, the most notable being Fcγ receptor-mediated phagocytosis where Fcγ receptors form ligands with antibody (IgG) that propagates an "eat" signal. Advanced microscopy and image analysis pipelines enable the acquisition of volumetric timeseries with diffraction-limited resolution and with sufficient temporal resolution to quantify membrane dynamics. Through advanced microscopy of phagocytosis significant progress in the field has been made. The Mines Bioimaging group has been particularly interested in the interpretation of how "don't eat" signaling by CD47 influences target engulfment and the macrophage membrane dynamics during phagosome formation. Using antibody-labeled *O. aries* erythrocytes as targets exclusively displaying "eat" signals, we show that the macrophage lamella wraps tightly around the target and additional membrane protrusions develop nearby the forming phagocytic cup. Additionally, a local transient increase in membrane ruffling activity occurs local to the site of internalization. Substituting erythrocyte species with *M. musculus* erythrocytes incorporates species-matched "don't eat" signals alongside previous "eat" signaling during phagocytic events performed by murine derived macrophages. These insights into the methodology of how target presenting CD47 changes the phenotype of our phagocytic cup and elaborates on this molecule's relevance in phagocytosis.

Improving the performance of $LiFePO_4$ cathode by hetero-atom doping

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Ionic diffusivity plays a central role in the performance of the batteries. A cathode material $LiFePO_4$ (LFP) performs poorly at a high current rate due to low ionic diffusivity. Increasing its ionic diffusivity is essential to enhance its performance for its application in high-power density batteries required for hybrid and electric vehicles. Here, we use molecular dynamics simulations with machine learning force field (MLFF), and nudged elastic band (NEB) calculations to show that Li-ion diffusivity in LFP increases when doped with transition metal dopant Ru. This increment is accompanied by changes in lattice and its electronic properties, including reduction of lattice in the diffusion direction, appearance of defect states in the middle of band gap and vicinity of the conduction band, and reduction in Li-diffusion barrier. Our calculation informs parameters that affect ionic diffusivity in LFP, which may be used for machine learning-based materials design protocols.

Particle Identification for proton and pion simulated events discrimination using SuperFGD prototype detector.

Diana Leon Silverio, Physics
Dr. David Martinez Caicedo, Physics

The T2K (Tokai to Kamioka) is a long-baseline neutrino oscillation experiment in which a muon neutrino beam is produced by using the accelerator facility at Japan Proton Accelerator Research Center. T2K uses Super-Kamiokande as the far detector to measure the neutrino oscillation, and near detectors to study the neutrino beam just after its production. The T2K experiment has achieved major milestones in the study of neutrinos oscillations, and novel upgrades to its near detector complex are underway.

A novel three-dimensional projection scintillator tracker, called SuperFGD, is one of the key components of the ND280 near detector upgrade of the T2K experiment. The SuperFGD detector will be made of optically-isolated scintillator cubes of 10x10x10 mm3. Due to the fine granularity and good timing resolution, the SuperFGD detector will provide valuable data for studying neutrino interactions. A prototype of the SuperFGD detector of 24x8x48 cubes was exposed to a neutron beam at Los Alamos National Laboratory (LANL) to study the detector's response to neutrons. This talk will present preliminary results on the implementation of particle identification (PID) tools for discriminating proton and pion using the SuperFGD prototype detector simulation. This PID development will allow future neutron-induced proton and pion production cross-section measurements on the scintillator using the SuperFGD prototype data.

Time Dependent Detector Signals for Improving Dark Matter Searches

Jack Genovesi, Physics Department
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The theory of Weakly Interacting Massive Particles (WIMPs) provides an attractive dark matter candidate particle which is currently being sought at the LUX-ZEPLIN (LZ) Dark Matter Experiment underground at Sanford Lab in Lead, SD. This theory attempts to explain the observed faster than expected galactic rotation of stars further away from the center by introducing massive amounts of dark matter in the halo. Dark matter would be comprised of relatively massive neutral particles that interact gravitationally but not electromagnetically. These so-called WIMPs that cannot be “seen” and are therefore referred to as “dark matter.” LZ is an ultra-quiet two-phase xenon time projection chamber with an active mass of 7 tonnes, which can observe even very rare radioactive decay events and hopefully discover WIMPs. An anticipated unique feature in the galactic WIMP signal compared to background noise, such as radioactivity, will be the annual modulation of the WIMP flux. This seasonal variation is due to the Earth’s orbit around the sun, in which Earth will be going into or with the WIMP wind. We present a study of this unique feature in the potential identification of WIMPs. The smallness of the effect clearly warrants the careful study of other time dependent backgrounds and detector conditions, such as the lifetime of signal electrons in our detector.

Modeling the Path of Rn-222 Decay Daughters in the LZ TPC

James Haiston, Physics Department

Dr. Richard Schnee, Physics Department

95% of the universe consists of things we cannot see and do not understand well. The LUX-ZEPLIN (LZ) collaboration is attempting to detect and add to our understanding of dark matter, which makes up ~27% of the universe. Interactions from radon-chain decays may be mistaken as a dark matter signal in the LZ detector. By understanding the path of radon-chain atoms in the liquid xenon (LXe) of the LZ detector, we can predict the locations of their interactions and hence discriminate them from potential signals caused by dark matter. The path of these atoms is complicated, depending on convective fluid flow in the LXe, the charge state of the atom in the detector's strong electric field, and whether the atom has combined to form a heavier (and slower) charged molecule. I am working to develop algorithms to determine quantities important for modeling the atom flow from LZ data. I will calculate the fraction of radon daughters that are charged, the mobilities of charged atoms mu_{+} and molecules mu_{m}, and the mean time for charged atoms to combine (τ_C) or neutralize (τ_N). Determining quantities that describe the atom flow will help the development of algorithms to identify the radon-chain interactions in LZ data, greatly improving the sensitivity of the search for dark matter.

Magnetic Phases of Semiconducting CrI_2 Monolayer

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The recently discovered van der Waals magnetic semiconductor CrI_2 shows promise for spintronic applications. Using density functional theory (DFT) calculations, we show that the CrI_2 appears at the low Iodine concentration in the Cr-I phase diagram. We find that the magnetic ground state is antiferromagnetic (AFM) with a large magnetic moment (~ 4.0 μB/Cr). Both structural phases (orthorhombic and monoclinic) have similar electronic properties and have a sizable thickness-dependent band gap. Further, we show that single layers of CrI_2 are dynamically and thermally stable at room temperature and can be easily exfoliated because of the low cleavage energy (~ 0.25 J/m^2), similar to CrI_3. Using the first and second nearest exchange interactions obtained by mapping DFT with Heisenberg Hamiltonian, we construct a magnetic phase diagram of a single layer, including all the phases competing with the ground state AFM phase. We find a way to achieve an antiferromagnetic to ferromagnetic transition through strain and/or hole doping. Hence, our work contributes to understanding the CrI_2 monolayer and its applications in spintronic devices.

Atomistic Structures of Temperature Dependent Thermal Expansion in Amorphous Multi-Component Metal Alloys

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Dr. Nickolaus Bruno, Mechanical Engineering Department
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The thermal expansion coefficient (TEC) of 72.5Fe-1Cu-2W-2Nb-15.5Si-7B (at%) and 69.5Fe-6W-6Nb-19.5B (at%) is calculated using density functional theory calculations (DFT). To achieve long simulation times, we develop a technique to generate machine learned force fields (MLFF) by fitting DFT forces and energy. The MLFF is validated using 72.5Fe-1Cu-2W-2Nb-15.5Si-7B (at%) composition with a known TEC. Using the same techniques, we generate a new force field for 69.5Fe-6W-6Nb-19.5B (at%) composition and predict the TEC. Two phase transitions were found to occur between 200-400K. To understand the origin of these transitions, we analyze the evolution of magnetic moments and local atomic structures using Voronoi analysis. Both transitions are found to be amorphous structural phase transitions associated with vertex sharing clusters.