

Manitoba Materials Conference 2017

May 9th, 2017 Engineering & Information Technology Complex Atrium

Poster Abstracts

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Materials Chemistry
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The abstracts contained within the document represent a selection of work undertaken within MIM over the last year. This internal document is not intended for publication or dissemination.

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Systematic Studies Of Electronic Structures And MCD Spectra Of Synthetic Oxochlorins, Dioxobacteriochlorins, And Dioxoisobacteriochlorins

Presented by: Dustin Nevenon

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Advisor(s): V.N. Nemykin

Co-Author(s): Elizabeth Kaesmann, Ruoshi Li, Christian Brückner, Victor Nemykin

Research Area(s): Complex Natural Systems

Due to their near infrared (NIR) absorption within the optical window of tissue, hydroporphyrins are appropriately suitable for their application as imaging agents in biological tissue or photochemotherapeutics (1). Oxidative modification of the β -pyrrolic positions in octaethylporphyrin (OEP) results in the formation of the oxochlorins, dioxobacteriochlorins, and dioxoisobacteriochlorins which possess more intense NIR absorption bands than the parent porphyrin (2). Although long known, their electronic structures have not been comprehensively described. Insight into electronic structure of these compounds was gained using magnetic circular dichroism (MCD) and UV-Vis-NIR spectroscopic studies, coupled with Density Functional Theory (DFT) and Time-Dependent DFT (TDDFT) calculations. Both theoretical and experimental methods suggest that all hydroporphyrin analogues analyzed exhibit a rare $\Delta\text{LUMO} > \Delta\text{HOMO}$ relationship of their frontier orbitals typically observed in naturally occurring chlorins, such as the chlorophylls. This characterizes the synthetic oxochlorins as true hydroporphyrin analogues (2).

1. Inhoffen, H.H.; Nolte, W. *Liebigs Ann. Chem.* 1969, 725, 167-176.

2. Rhoda, H.; Akhigbe, J.; Ogikubo, J.; Sabin, J.; Ziegler, C.; Brückner, C.; Nemykin, V. *J. Phys. Chem. A*, 2016, 120, 5805–5815.

Phase Stability Of Natural Colloidal Systems Measured By Dynamic Sound Scattering

Presented by: Anatoliy Strybulevych

Researcher at the University of Manitoba, Department of Food Science

Advisor(s): M Scanlon

Co-Author(s): Tomohisa Norisuye, Nikolay Repin, John Page, Martin Scanlon

Research Area(s): Complex Natural Systems

In this poster we show how Dynamic Sound Scattering (the acoustical analog of Dynamic Light Scattering) is used to study diffusion and sedimentation of submicron particles in a natural colloidal system - milk. Milk is a semi-dilute dispersion (volume fraction of ~ 0.11) of hard spheres (casein micelles with mean radius of ~ 100 nm) in a continuous phase containing water, lactose, salts and whey proteins. It is nutrient rich although it contains no fiber. We show that milk enriched with dietary fibers (barley polysaccharide β -glucan) is stable below a critical fiber concentration. Above it, there is rapid separation of the casein micelles driven by depletion flocculation. Sizes of the particles in both stable and non-stable phases are estimated using time-correlation functions.

Gas Assisted Extrusion As A Tool To Puff Snack Foods

Presented by: MengYuan Zhang

Undergraduate student at the University of Manitoba, Department of Food Science

Advisor(s): F. Koksel

Co-Author(s): Tugrul Masatcioglu, Filiz Koksel

Research Area(s): Complex Natural Systems, Soft and Disordered Materials

Extrusion is an efficient thermo-mechanical technique that combines blending, shearing and cooking operations. An extruded snack owes its appeal to its texture which is highly correlated to its aerated structure. Due to shifting consumer trends in the last couple decades, in addition to textural properties nutritional quality is becoming more important. Pulses are important sources of high quality proteins while being low in calories and glycemic index; providing tremendous opportunities to be used in various foods. In this study, the effects of extrusion cooking methods (with or without nitrogen injection) on physical properties of extruded snacks were investigated. Extruded snacks were made from yellow pea flour (26% protein) and water using a laboratory-scale twin-screw extruder. In both extrusion methods, die exit temperature, product moisture content, screw speed, and die diameter were: 150°C, 14%, 200 rpm, and 2.3 mm, respectively. During nitrogen assisted extrusion, three injection pressures (3, 4 or 5 bar) were studied, through a pressure regulator attached onto the extruder barrel. Compared to conventional extrusion, nitrogen injection (at all pressures) significantly affected the aerated structure of the extrudates, i.e., more homogeneous cell structures were generated with nitrogen. As nitrogen injection pressure increased from zero to 3, 4, and 5 bars, extrudate expansion index decreased while extrudate bulk density increased. Our results demonstrate that the physical properties of extrudates can be controlled by manipulating nitrogen injection pressure during gas assisted extrusion, opening food industry's doors to production of snacks with a spectrum of shapes and sizes.

Use Of Air-Coupled Ultrasound Transducers To Characterize White Salted Noodle Dough

Presented by: Huiqin (Mia) Wang

MSc Candidate at the University of Manitoba, Department of Food Science

Advisor(s): M Scanlon

Co-Author(s): Reine-Marie Guillermic; Sébastien Kerhervé; Anatoliy Strybulevych; John Page; Martin Scanlon

Research Area(s): Complex Natural Systems, Soft and Disordered Materials, Composite Material Systems

Noodle dough is made from wheat flour, water and salt, and its consistency is the key to ensure a smooth processing operation, a uniform gluten development and an optimal eating quality. Wheat flour dough is a heterogeneous composite soft material, and its mechanical properties can change considerably during processing operations. Therefore, capturing the mechanical properties of dough is a great challenge. In this study, two air-coupled ultrasound transducers (central frequency: 225 kHz) were used as a materials characterization tool. Measuring the phase velocity and attenuation coefficient of ultrasonic waves traveling in the sample allows calculation of the longitudinal mechanical properties, and therefore can help to understand the dynamic physiochemical changes that occur within the dough during processing. In this study, noodles were formulated with CWRS (Canadian Western Red Spring) at two different water levels (32% and 36%). Noodle with 36% water showed a lower phase velocity and higher attenuation coefficient, indicating a plasticizing effect of water in the noodle dough system. As the work input to the dough increased during the sheeting process, the phase velocity of both samples increased slightly. But dramatic changes occurred 24 hours after noodle processing. The phase velocity of aged noodles almost doubled. This could be due to a structural modification of gluten polymers and starch in the dough matrix or/and a change in the size and distribution of trapped air bubbles.

Analysis Of Dew Retting Of Hemp And Flax In Manitoba

Presented by: Jean-Christophe Habeck

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Advisor(s): J Morrison

Co-Author(s): Tasneem Vahora, Shawna DuCharme, Diogenes Vedoy, Lin-P'ing Choo-Smith

Research Area(s): Complex Natural Systems, Soft and Disordered Materials

The use of fibre from hemp and flax straw in composites and textiles requires that the ligno-cellulosic material be separated from the portions containing hemi-cellulose or other tissues. This is traditionally done after "water-retting"; that is, submersion in water to promote anaerobic digestion of non-cellulosic plant tissue. A less polluting/water expensive method is to allow stems to lay in the field and "dew-ret". This work examines the efficacy of dew retting in Manitoba versus "water-retting" and unprocessed hemp and flax. Specific outcomes examined are the fibre yield, qualitative microscopic texture analysis, and compositional content of fibre through bulk attenuated total reflection in Fourier Transform InfraRed analysis of fibre.

Flax and Canola Stem Cross-Section Preparation for FTIR Spectromicroscopy

Presented by: Tasneem Vahora

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Advisor(s): J Morrison

Co-Author(s):

Research Area(s): Complex Natural Systems, Soft and Disordered Materials

The analysis is performed in the mid-infrared (mid-IR) region ($900\text{cm}^{-1} - 4000\text{cm}^{-1}$) using an fourier transform infrared (FTIR) spectromicroscope. The goal of this preliminary research is to develop a method for sample preparation that results in FTIR data for determination of chemical distribution without interference of embedding materials or other process alterations to the samples. FTIR spectromicroscopy is a chemical imaging technique that aids in the determination of chemical compositional distribution throughout the anatomy of the stem. This methodology has been successfully applied in previous research involving flax to identify the primary chemical constituents in the stems (i.e., cellulose, hemicellulose, lignin, pectin and wax). The dried and rehydrated stems of flax and canola were imaged using FTIR transfection mode. Samples for cross-sectioning are embedded in media, then frozen, microtomed to approximately $5\text{-}20\mu\text{m}$ thickness and mounted on a MirIR slides (coated with IR reflective material) for transfectance FTIR. The maps of chemical compositional distribution obtained from flax stems provide correlation with location of fibre bundles determined. The results indicate that due to the differences in fragility of dried stems that while flax cross-sectioning was successful the canola cross-sectioning was not successful and remains an elusive task.

Monitoring Of Damage Progression In Glass Fiber Reinforced Polymer Rods Using Acoustic Emission Entropy

Presented by: Mohammadhadi Shateri

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Advisor(s): Dr. Thomson

Co-Author(s):

Research Area(s): Composite Material Systems

Glass fiber reinforced polymer (GFRP) rods have been widely used in reinforcing of the civil structures. High strength-to-weight ratio and high resistance to the corrosion make the GFRP rods a good replacement for steel reinforcing rods in civil engineering applications. The GFRP rods can become damaged due to excessive loading or accidental sources of damage. According to the CAN/CSA-S806-12 standard, the maximum recommended stress in GFRP rods under service loads should not exceed 25% of the ultimate strength. This stress value is set to prevent creep failure in GFRP bars. However, for in-service applications there are few physical indicators that this value has been reached or exceeded. In this work analysis of acoustic emission (AE) signals in frequency domain is used to determine when the maximum recommended stress in GFRP rods has been exceeded.

Synthesis Of Bulk Metallic Crystalline-Amorphous Composites

Presented by: Taiwo Dada

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Co-Author(s): Chuang Deng, Olanrewaju Ojo

Research Area(s): Composite Material Systems

Materials with microstructural heterogeneity have recently attracted dramatic attention in the materials science community to achieve both high strength and ductility. In the present study, Accumulative Roll Bonding (ARB) was used to process a composite of copper and a nickel based metallic glass. By using optical microscopy, rupture of the hard-metallic glass phase was detected even after one cycle. Cu/MG sheets were seen to have deformed inhomogeneously, accompanied by the formation of multiple fracture of the MG layers. These fractured fragments of the MG layers were then distributed in the Cu matrix. Further ARB passes show that some of the metallic glass fragments are ruptured into tiny pieces and distributed more homogeneously in the crystalline copper matrix.

Sensitivity Analysis Of A Parallel Plate Method For Measuring The Dielectric Permittivity Of High Voltage Insulating Materials

Presented by: Anton Vykhodtsev

MSc Candidate at the University of Manitoba, Department of Electrical and Computer Engineering

Advisor(s): D.R. Oliver, B. Kordi

Co-Author(s): D.R. Oliver, B. Kordi

Research Area(s): Composite Material Systems

Dielectric frequency response characterization of polymeric insulation materials is often used to perform comparative studies of ageing in case of samples from the decommissioned installations or obtained employing accelerated ageing in the laboratory environment. Particular interest for this analysis presents a low frequency range since noticeable markers of ageing such as interfacial charge dynamics, new localized charge sites, and pure DC conductivity are detected. This low frequency spectroscopy may be conducted using the sample fixture/holder in the form of a parallel plate capacitor. In the case of polymeric samples, the possibility of physical deformation within the sample holder and presence of the contact resistance between sample and plates add additional variability to comparative measurements. This work undertakes a systematic sensitivity analysis of a contact-free parallel-plate capacitance measurement approach for polymeric materials that only has one capacitance plate in contact with the sample, avoiding aforementioned issues. The analysis demonstrates that the uncertainty in the measurement of the dielectric constant and loss tangent mostly depends on the precision with which the plate-plate and plate-sample separation is determined. The measurements also show that the determination of loss tangent can be susceptible to uncertainties arising from electrical noise, but that these can be controlled further by utilizing more refined instrumentation.

Comparison Between Microstructural Analysis Of FRP Bars Using Micro Computed Tomography (μ ct), Scanning Electron Microscope (SEM) Techniques

Presented by: Maha Ghaib

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Advisor(s): D. Svecova, D. Thomson

Co-Author(s): Mohammadhadi Shateri, Michael Jackson, Ravinder Sidhu, Douglas J. Thomson , Dagmar Svecova

Research Area(s): Composite Material Systems, Mechanics of Materials and Structures

Fiber reinforced Polymer (FRP) bars have linear-elastic behavior up to failure. Therefore, new methods are being investigated to determine the level of damage in these bars at various stages of loading. The aim of this study is to evaluate the micro computed tomography (μ CT) as a tool to study the changes in the internal structure of different Carbon Fiber Reinforced Polymer (CFRP) and Glass Fiber Reinforced Polymer (GFRP) rebars subjected to tensile loading at different percentage of the ultimate load and to confirm the μ CT results by using scanning electron microscope (SEM) technique.

Microcracks and voids were examined, and the damage thickness and distribution as well. GFRP bars revealed more damage comparing to CFRP bars for the same diameter. Damages are mostly started in the voids regions and expanded along the samples lengths for both GFRP and CFRP samples. The image slices revealed that the voids and cracks are increased with the increasing of the ultimate load, and the increasing started approximately after 40 % of the ultimate load in GFRP and after 50% of the ultimate load in CFRP. The analysis of FRP bars by μ CT opens up the possibility of tracking changes in the FRP bars internal structure as a result of tensile loading.

Size Dependent Strength And Plasticity In Nanocrystalline Metals With Amorphous Grain Boundary

Presented by: Afzal Hossain Neelav

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Advisor(s): Chuang Deng

Co-Author(s): Chuang Deng

Research Area(s): Composite Material Systems, Crystalline Materials and Nanostructures

Grain boundaries play a significant role in polycrystalline materials as they control the overall microstructural evolution and serve as both sinks and sources for dislocation activities in the material. By replacing crystalline atoms at the grain boundary region with amorphous interfacial films, it is possible to enhance dislocation absorption and so, reduce crack nucleation and growth at the interface. In this study, molecular dynamics simulations are used to investigate the interface energy of bicrystal and polycrystal Cu with amorphous interface, their deformation mechanism under shear and tensile loading. It is found that refining the grain size can have a great impact on the strength and plasticity of the metals which has been usually established by the Hall-Petch relationship. Therefore, it is interesting to study the effects of both the grain size and interface thickness on the strength of nanocrystalline Cu with amorphous interface and find out if the Hall-Petch relationship still holds in this novel type of materials.

Non-Spherical Magnetic Nanoparticles For The Treatment Of Infection

Presented by: Rachel Nickel

MSc Candidate at the University of Manitoba, Department of Physics and Astronomy

Advisor(s): J. van Lierop

Co-Author(s): J. Li, P.K. Manna, S. Liu

Research Area(s): Crystalline Materials and Nanostructures, Composite Material Systems

Microbial resistance is a global healthcare crisis. Topical biocides are a possible solution; however, because they do not have specific targets, cytotoxicity is a problem if the biocide remains in contact with the host. By biocide-coating magnetic nanoparticles we obtain a system that may be removed using an external magnetic field, thus limiting contact time. Spherical iron oxide nanoparticles (3 nm and 8 nm in diameter) coated with a QAC biocide have been proven effective against both MRSA and *P. aeruginosa*, but are difficult to remove from wounds. This research examines non-spherical iron oxide nanoparticles to determine an optimal size and shape. Nanoparticles were synthesized using single-ion precipitation at various temperatures resulting in Fe₃O₄ disks, cubes and polyhedra. After characterization using XRD, TEM and SQUID magnetometry, the nanoparticles were coated with SiO₂ and functionalized with a N-chloramine biocide. Biological tests performed on MRSA show the efficacy of the systems varies with particle shape.

Monte Carlo Study Of A Geometrically Frustrated Rare Earth Compound: SrGd₂O₄

Presented by: Emrul Hasan

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Advisor(s): B. Southern

Co-Author(s): B. W. Southern

Research Area(s): Crystalline Materials and Nanostructures

We study the low temperature magnetic phase transitions and phase diagram of one member of the lanthanide family of frustrated compounds, SrGd₂O₄, using Monte Carlo simulation techniques. Frustrated magnetism is the study of competing interactions between the neighbouring spins. Recently, frustration has been identified in a rare earth family of compounds with the formula SrLn₂O₄ where Ln=Ho, Gd, Er, Dy, Tm, and Yb.

The two dimensional honeycomb structure of SrLn₂O₄ in the ab plane is connected by triangular chains running along the c direction, making the system frustrated. We have used a model of classical Heisenberg spins to investigate the low temperature behaviour. We have studied the cases of pure exchange and pure dipole interactions as well as their combined effects. Our simulation results qualitatively agree with the experimental findings.

The Magnetic Properties Of CoFe₂O₄ Nanoparticles With Cubic Anisotropy

Presented by: Çiğdem Elif Demirci

Researcher at the University of Manitoba, Department of Physics and Astronomy

Advisor(s): J van Lierop

Co-Author(s): Johan van Lierop, Selçuk Aktürk, Palash Manna

Research Area(s): Crystalline Materials and Nanostructures

Cobalt ferrite, CoFe₂O₄, is of particular interest because it has strong multiaxial (cubic) magnetocrystalline anisotropy that leads to a more complex system of energy barriers which is also related to heating efficiency of the system. How the heating efficiency is determined by the intrinsic magnetic properties like the magnetocrystalline anisotropy is an open question.

In this study, .18 nm CoFe₂O₄ nanoparticles have been prepared using a non-aqueous solvothermal method. We have found that the thermal variations of the saturation magnetization in the temperature range 200-400 K follows a modified Bloch's law that shows a threshold thermal energy is required to generate spin waves. The deviation from the model at low temperatures can be explained by the strong interparticle interactions that dominate the system. The large magnetocrystalline anisotropy obtained leads to these particles potential application as effective magnetic hyperthermia. The study of the different magnetic properties in CoFe₂O₄ nanoparticles with the substitution of rare earth elements (La⁺³ and Gd⁺³) in place of Fe⁺³ ions is underway currently. We aim to provide a better understanding of the physics behind the effective heating of doped and undoped CoFe₂O₄ nanoparticles, focusing on the role of effective magnetic anisotropy that strongly depends on cation distribution due to the preferred occupied positions of rare earth ions.

This work was supported by the Scientific and Technological Research Council of Turkey (TUBİTAK).

Breaking The Second Law Of Thermodynamics? Proteresis In Cube Shaped Co_3O_4

Presented by: Michael Shepit

Undergraduate student at the University of Manitoba, Department of Physics and Astronomy

Advisor(s): J van Lierop

Co-Author(s): Dr. J. van Lierop

Research Area(s): Crystalline Materials and Nanostructures

Regarding the second law of thermodynamics, the entropy of a system can only increase (or at best, stay the same) over time. A hysteresis loop is caused by the dissipation of energy which is calculated by the area inside the loop. Cobalt oxide (Co_3O_4) is used in a wide variety of fields, from catalysis to energy storage applications. In this work, three different morphologies of Co_3O_4 were synthesized (two nano-sized systems and a bulk system). Two distinct shapes were obtained: cubes (side length: 15 nm) and hexagonal plates (diameter: 73 nm, thickness: 9 nm). X-ray diffraction, transmission electron microscopy, and SQUID magnetometry were used to characterize the samples. Bulk Co_3O_4 is an anti-ferromagnet with a normal spinel crystal structure. The plates and the cubes both display unusual ferromagnetic-like behaviour below the magnetic ordering temperature. Hysteresis loops for the hexagonal plates show a large anisotropy due to the shape of the particle. The magnetometry measurements performed on the cubes show a strange magnetic behaviour known as proteresis. This causes the hysteresis loop to appear upside down and this process seems to violate the second law of thermodynamics.

Spectroscopic Studies of A New Azido Bridged Ni(II) Complex, di- $\mu_{1,1}$ -azido- $\kappa^4 N:N$ -bis{ethanol[2-hydroxypropylimino)methyl]-3,5-chlorophenolato- $\kappa^3 N,N',O$ }-nickel(II)

Presented by: Adem Dönmez

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Advisor(s):

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Research Area(s): Crystalline Materials and Nanostructures

Ni(II) complexes have attracted much attention during recent decades owing to their interesting architectures and potential applications in fields such as coordination polymers, magnetochemistry, bioinorganic chemistry and dye-sensitized solar cells (DSSCs). In this study, a new double end-on azido-bridged dinuclear Schiff base nickel(II) complex, $[\text{Ni}_2(\mu_{1,1}\text{-N}_3)_2(\text{HL})_2(\text{EtOH})_2]_2$, **1**, [**HL**=2-[(2-hydroxypropylimino)methyl]-3,5-chlorophenol] has been synthesized and characterized by elemental analysis, UV and IR spectroscopy, single crystal X-ray diffraction methods. Complex **1** crystallizes in triclinic space group, *P*-1. The compound contains half of the two dinuclear azido bridges $[\text{Ni}_2(\mu_{1,1}\text{-N}_3)_2(\text{HL})_2(\text{EtOH})_2]$ molecules in the asymmetric unit. The Ni(HL) units in each dinuclear molecule are connected to each other by two bridging end-on azide ligands. Each Ni(II) atom is six-coordinated by the ONO donor set of the Schiff base ligand and by one terminal N atom of one bridging azide ligand, defining the basal plane, and by one terminal N atom from the other bridging azide ligand and one donor O atom from the EtOH molecule occupying the axial positions, forming a distorted octahedral coordination. In the crystalline architecture of complex **1**, intermolecular O-H \cdots N and C-H \cdots N hydrogen bonds link the molecules which form a two-dimensional structure. The electronic spectrum of the free ligand (**HL**) shows a high broad absorption band and this arises process may be due to the conjugated systems. On the contrary, it has been seen two different absorption bands in the UV spectrum of complex **1**. These absorption bands can be attributed to the $n \rightarrow \pi^*$ or $\pi \rightarrow \pi^*$ electronic transition for the lower one and can be attributed to the $d \rightarrow d$ transition for the higher one, respectively. The IR spectra of the free ligand (**HL**) show a broadband in the high frequency region and attributes to $\nu(\text{O-H})$ stretching, which is disappeared in complex **1** indicating deprotonation of the phenolic hydroxyl group upon complexation. The several weak peaks in the range of intermediate frequencies are likely to be due to the characteristic aromatic and aliphatic $\nu(\text{C-H})$ vibrations for the ligand and complex **1**. The IR spectra of the free ligand show the strong absorption band in the lower frequencies which is attributed to the characteristic $\nu(\text{C=N})$ stretching.

Understanding The Structure And Properties Of The $\text{Sc}_2\text{O}_3 - \text{V}_2\text{O}_3$ Phase Diagram

Presented by: Joey Lussier

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Research Area(s): Crystalline Materials and Nanostructures

Fuel cells are vital technologies for the future of alternative energy due to their fuel flexibility, low emissions and high conversion efficiency. Ion conductors as solid-state electrolytes play a crucial role in improving alternative energy conversion devices. Shafi, et al.[1,2] showed that the structural relationship between the bixbyite and fluorite structures permits control of oxidation states and oxygen defects (A=Sc,In; B=Ti,V). Some problems that arose in these systems include that the defect fluorite $\text{ScVO}_{3.7}$ undergoes a non-topotactic (reconstructive) oxidation and results in the formation of an ordered zircon structure. This oxidative transition occurs below the typical operating temperature of solid oxide fuel cells (SOFC) and will destroy the solid state electrolyte. In order to stabilize the defect fluorite and avoid a phase transition to a zircon structure up to the operating temperatures of SOFCs, the full $\text{Sc}_2\text{O}_3 - \text{V}_2\text{O}_3$ phase diagram will be presented. Furthermore, recent results in oxide anion substitution with halides as a means of defect fluorite stabilization will be discussed. We report synthesis, structural characterization using X-ray and neutron scattering, thermal analysis, ion conductivity measurements, and reactivity studies using in-situ x-ray diffraction.

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Towards A'A''VO₅ Phases Using Solid-State Paths

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Research Area(s): Crystalline Materials and Nanostructures

Contemporary hydrocarbon fuel infrastructure has a demand for conversion-effective, durable, and space-saving routes of oxidant delivery. Solid-state oxide fuel cells (SOFCs) meet these requirements in full. Ideal SOFCs are powder-based electrolytes with high O²⁻ mobility due to randomization of oxygen vacancies and weak bonding between lattice cations and oxide anions. Well-known SOFCs, however, operate at considerably elevated temperatures - 1000 °C [Goodenough, 2015]. Much lower temperatures may be achieved for phases like A³⁺₂V⁴⁺O₅ (oxygen-defective MeO₂), which synthesis is one of the main goals of our research. Interestingly, known A₂VO₅ compounds have different symmetry, possibly due to different synthesis techniques. Thus, tetragonal Sc₂VO₅ was obtained by liquid phase coprecipitation synthesis with further single crystal growth [Cong, 2010], orthorhombic In₂VO₅ – by solid-state chemistry in vacuum [Möller, 2007], monoclinic Yb₂VO₅, Y₂VO₅, and Dy₂VO₅ – by low-temperature hydrothermal crystallization [Kimani, 2012], most part of A₂VO₅ compounds being the side products.

We made attempts to synthesize Lu₂VO₅ by solid-state approach, Lu³⁺ radius (0.861 Å) being between those of In³⁺ (0.800 Å) and Yb³⁺ (0.868 Å) known to form different symmetries. However, direct solid-state synthesis with VO₂, proposed for the case with Sc₂VO₅ [Mikhailov, 1971], and synthesis through vanadium comproportionation, including that via intermediate pyrochlore Lu₂V⁴⁺₂O₇, always led to stable zircon LuV⁵⁺O₄ and perovskite Lu³⁺VO₃ formation, as proved by powder XRD. This problem now is being addressed through enhancing of Lu₂O₃ activity with highly reactive In₂O₃, thus aiming at Lu_{2-x}In_xVO₅ formation. The same approach is being applied to get Y_{2-x}In_xVO₅ and Yb_{2-x}In_xVO₅, also never obtained by solid-state chemistry.

H-T Phase Diagram Of The 3D Kagome Lattice

Presented by: Daniel Maciel

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Research Area(s): Crystalline Materials and Nanostructures

Antiferromagnetism is a type of magnetism that exhibited in certain materials and has long been a subject of interest for researchers in the field. At low temperatures in antiferromagnetic materials the spins in the lattice must align themselves in an anti-parallel configuration between their neighbours to minimize their exchange energy in their ground state. Complications arise when the lattice is composed of triangles as the exchange energy cannot be mutually satisfied between neighbours on the lattice. This phenomena is called geometric frustration and leads to interesting ground state configurations.

While there have been many studies done on geometrically frustrated lattices in two dimensions, research on the subject in three dimensions has yet to be explored fully. Therefore this paper will seek to develop an H-T phase diagram a specific type of triangular lattice type called the Kagome lattice which is observed in some real materials such as IrMn_3 .

To characterize these transitions standard heat bath Monte Carlo simulations for a number of different lattice sizes will be performed with magnetic spins being distributed on each site according to a Boltzmann Distribution. A variety of order parameters such as spin stiffness, correlation length and magnetic susceptibility will be measured as these quantities experience measurable changes at or near transitions.

This project will seek to illuminate the effects of geometrical frustration in three-dimensions and compliment previous work done on this topic in two-dimensions

Understanding NMR Spectra Of Paramagnetic M(acac)_x Complexes In The Solid State

Presented by: Kirill Levin

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Research Area(s): Crystalline Materials and Nanostructures

To facilitate applications of NMR to paramagnetic solids, we use fast Magic Angle Spinning (MAS) in conjunction with Density Functional Theory (DFT) to analyze electron spin density distributions in well-characterized metal-acetylacetonate coordination compounds. DFT proves to be remarkably effective in predicting peak positions, making signal assignments relatively straightforward. Spin-density contour maps provide valuable insight into the mechanisms underlying the observed ¹³C and ¹H peak shifts. Peak widths are differentially affected by electron relaxation and shown to be informative for the estimation of electron-nuclear interactions. This approach permits optimization of NMR experiments and offers chemists an additional tool for extracting structural information.

One-Pot Synthesis Of Amine-Functionalized Fe₃O₄ Nanodiscs And Their Sample Biomedical Applications

Presented by: Palash Manna

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Advisor(s): J. van Lierop

Co-Author(s): R. Nickel, Y. Wroczynskyj, V. Yathindranath, Jie Li, Song Liu, D. W. Miller, and J. van Lierop

Research Area(s): Crystalline Materials and Nanostructures

Magnetite (Fe₃O₄) nanoparticles coated with a suitable biocompatible material can have various applications as in targeted drug delivery, hyperthermia, and topical biocide application and removal. The innate biocompatibility of Fe₃O₄ (also approved by the FDA) makes it the most sought-after candidate for such purposes. The morphology, aspect ratio and orientation of the nanoparticles influence their interaction with biological systems. We have found previously that non-spherical nanoparticles have an improved cellular uptake profile compared to spheres. However, synthesis of non-spherical nanoparticles often involves multiple reagents, several steps and a highly controlled environment.

We have found a new way of synthesizing non-spherical Fe₃O₄ nanoparticles in gram-scale quantities which does not involve (i) multiple steps (one-pot reaction) and (ii) multiple reagents (just two reagents; iron(II) chloride tetrahydrate and triethylamine) and (iii) elevated temperature (can be done at room temperature) and (iv) controlled environment (was done in an open beaker). Using x-ray diffraction and Mössbauer spectroscopy techniques, we have tracked the reaction path, quantified the amount of intermediates present, and proposed the chemical reaction pathways. By modifying the surface further with bicides and EDTA-Na₃ (N - (trimethoxysilyl- propyl)ethylenediaminetriacetate trisodium salt), we have shown that these nanoparticles (i) are 100% effective in inactivating methicillin-resistant staphylococcus aureus (MRSA) bacteria in 2 hours, and (ii) have 100% cellular uptake profile in presence of a small dc-magnetic field, making them a promising candidate as drug carriers for magnetic field targeted delivery.

Helping Solve The Rare Earth Crisis: Crystalline Iron Cobalt Nanoparticles For Use In Hard/Soft Nanocomposites

Presented by: Kelly Newman

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Research Area(s): Crystalline Materials and Nanostructures

Soft magnetic materials like iron cobalt are ideal for transformer and inductor cores due to high saturation magnetization and low hysteretic losses. Iron cobalt is an alloy of two non-rare earth elements that are relatively accessible and therefore, inexpensive. The bulk alloy has a saturation magnetization higher than any other rare-earth free system. When iron cobalt nanoparticles are synthesized using a scalable metal halide reduction, 4 nm particles are produced. Mossbauer spectroscopy, x-ray diffraction (XRD), x-ray absorption (XAS) and x-ray magnetic circular dichroism (XMCD) all confirm the amorphous nature of these particles. These particles are then annealed at 450 C to achieve 25 nm particles. These particles exhibit a highly crystalline structure which is confirmed by XRD and refinement of these XRD patterns a temperature dependence of the lattice volume. The 25 nm iron cobalt nanoparticles also have a temperature dependent coercivity. This is indicative of the magnetic anisotropy of the particles. The dependence of the anisotropy on the lattice volume will be discussed as well as the other factors that contribute to magnetic anisotropy.

Dipolar Ferromagnetism In Three-Dimensional Superlattices Of Nanoparticles

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Advisor(s): J. van Lierop, B.W. Southern

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Research Area(s): Crystalline Materials and Nanostructures

Atomistic core-shell models of maghemite spherical nanoparticles and three dimensional hierarchical structure of these nanoparticles using newly developed stochastic Landau-Lifshitz-Gilbert (sLLG) simulations, are presented. Our simulations are able to correctly simulate real experiments on magnetic nanoparticles, such as the unusual temperature dependence of the magnetism χ an open question in the literature. We find that the atoms on the surface (radial surface anisotropy) gives rise to a surface magnetization with an unforeseen domain wall separating the magnetic poles of a spherical nanoparticle. The inhomogeneity of the oxygen ion distribution on the nanoparticle surface results in a pinning of this domain wall, and this pinning is shown to play an important role in the temperature dependent magnetism relaxation processes. In an face-centred cubic (FCC) superlattice of these nanoparticles, we confirm the postulate that dipolar interactions should permit a new type of ferromagnetism. Additionally, we find that the surface anisotropy pinning effect of the nanoparticles in a FCC superlattice decreases the alignment the nanoparticles' magnetizations, reducing the overall magnetism of the superlattice with decreasing temperature (e.g. 20 K for 7.5 nm nanoparticles with a 0.6 nm thick shell of disordered atoms) – as observed in experiment.

Nanoceria And NO_x Catalysis: The Missing Link To Predicting Catalytic Activity Is Quantifying The Dynamic Oxygen

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Research Area(s): Crystalline Materials and Nanostructures, Surfaces and Interfaces

Oxygen vacancy defects in nanoscale CeO₂ (nanoceria) are of special importance because of their impact on the structure and electronic properties of the surface. Nanoceria has attracted much attention due to its catalytic properties, and one of the critical aspects of this novel catalyst is its oxygen partial pressure dependent ability to undergo repeatable Ce⁴⁺-to-Ce³⁺ redox cycles through oxygen vacancy formation. Oxygen vacancy transport, i.e. mobility of oxygen in the fluorite lattice, is therefore of fundamental interest due to the reactivity of these vacancies once they reach the surface. The magnetic susceptibility of ceria is sensitive to the redox transformation of diamagnetic Ce⁴⁺ (4f⁰) to paramagnetic Ce³⁺ (4f¹ with S=1/2 and J=5/2), and here we demonstrate this as a new window to study the evolution of vacancies and migration of oxygen atoms from inside the ceria structure to its surfaces, probing the oxygen through its antiferromagnetic to paramagnetic transition at 50 K. In this work we introduce magnetometry as a novel technique based on the magnetic response of Ce³⁺ and molecular oxygen adsorbed on the surface of nanoceria and ceria-based catalysts that quantifies for the first time the number and type of defects (e.g. reduced Ce³⁺, lattice oxygen vacancies, and Frenkel pairs), and demonstrates that this information is the missing link that finally enables predictive design of NO_x catalysis in ceria-based systems, a critical reaction for emissions control.

Analyses Of Softening Behaviour In Wire-Arc Additive Manufactured ATI 718PLUS

Presented by: Gbenga Asala

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Co-Author(s): J. Andersson, O.A. Ojo

Research Area(s): High Temperature Aerospace Materials

Additive manufacturing (AM), the industrial version of 3D printing, has gain significant attention in the manufacturing industries in the last few years as production of parts requires improvement in terms of quality and costs reduction. The objective of this study is to analyse and determine the mechanism responsible for a detrimental softening in a recently developed aerospace superalloy, ATI 718Plus, processed by wire-arc additive manufacturing. The study involved theoretical calculations coupled with electron microscopy and spectroscopy analyses. Thermodynamic simulation results suggest that the softening behaviour is caused by reduction in both the re-precipitation kinetics and the extent of precipitation of the key strengthening phases of the alloy, due to the effects of elemental microsegregation that occurred during the AM process. The calculations further show that the softening problem can be eliminated through an appropriate use of post-process thermal treatment that enables adequate diffusion driven solute re-distribution. Interestingly, the predictions of the thermodynamic calculations are experimentally confirmed and the softening problem is eradicated by the use of a post-process thermal treatment.

Viscoelastic Behavior Of A Cylinder Filled With A Compressible Fluid

Presented by: Vahid Rabbani

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Research Area(s): Mechanics of Materials and Structures

There are number of mathematical expression for modeling the viscoelastic behavior of a continuous medium. Among which the Maxwell model is one of the simplest one to implement. It is simply based on a mass-dashpot system in series. The energy dissipation element is a linear, first order damper in rate form. The goal of the proposed study is to apply this model to already existing purely elastic model of a cylinder. The fundamental, effective model would be the kind of Navier equation with Lamé' constants in the rate form. An analytical approach is desirable in the frequency domain. Later on it is can be integrated to a more general temporal response of the system. The numerical result of such a model can provide valuable clues to understand the energy dissipation and dispersion behavior of the boundaries. The validity of the model shall be cross-checked against previously published studies as well as commercial numerical packages such as Comsol.

The Effects Of Crystal Orientation And Voids On Aluminium Nanocubes Under Uniaxial Tension Studied By Molecular Dynamics Simulations

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Research Area(s): Mechanics of Materials and Structures

Molecular dynamic simulations using Embedded Atom Method (EAM) potentials and LAMMPS code are performed to investigate the deformation behaviour of Al nanocubes along different crystallographic orientations under uniaxial tensile loading. The specimens are constructed with spherical voids to analyse their effect on damage evolution. Moreover, the effect of void size on the strength of Al nanocubes is also studied by deforming the nanocubes along [001], [111] and [011] directions. The simulation results shows that loading the Al nanocubes (without voids) in [001] direction resists plastic deformation much more than [111] and [011] directions and exhibits much larger value of ultimate strength as compared to other two cases. Besides, the simulations show that the presence of voids degrades the strength of Al nanocubes and this degradation is exacerbated with increase in the size of the void. Interestingly, the effect of void size on deformation is much more pronounced when Al is loaded along [001] and [111] directions relative to [011] direction. The deformation sensitivity of a loading direction to the presence of voids follows the order [001]>[111]>[011]. This is explained by the physical behaviour of stacking faults formed during loading. All observations made during the simulations are supported by the atomic configurations at different stages of deformation and stress-strain curves.

Finite Element Study Of Dominant Stimulus In Regulating Femur Bone Remodeling

Presented by: Yichen Zhang

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Advisor(s): YL Luo

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Research Area(s): Mechanics of Materials and Structures

Based on the Wolff's law, mechanical stimuli affect the formation of bone structure and its bone mineral density (BMD) distribution. There are a number of possible mechanical stimuli, for example, von-Mises stress, tensile stress, compressive stress and strain energy density (SED). It is not clear which is the dominant stimulus. The objective of this study was to determine the dominant stimulus that regulates femur BMD by iterative finite element simulations of Wolff's law.

Four finite element models of a femur initially had the same finite element mesh, the same uniform BMD and were affected by the same habitual physiological loading. In the following iterative simulations, BMD in each model was 'remodeled' by one of the four stimuli. The iterations were continued until the change of BMD in each model was smaller than a specified value. The dominant stimulus was determined by comparing the simulated BMD with that measured by clinical QCT (quantitative computed tomography).

The results showed BMD distribution in the finite element model regulated by SED was closest to QCT measured BMD, followed by von-Mises stress and then tensile stress and compressive stress. It is thus concluded that SED was the dominant stimulus in regulating femur BMD.

Bending Active Framed Fabric Formwork Structures

Presented by: Lancelot Coar

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Advisor(s): L De Laet, M West

Co-Author(s):

Research Area(s): Mechanics of Materials and Structures, Surfaces and Interfaces

This research explores the potential of flexible materials to create self-organizing structures to produce structurally efficient, buildable and unique architectural forms. Specifically, this work looks at the use of fiberglass rebar to create bending active (BA) frames as a structural framework to support fabric formwork. Once mounted to the BA frame, the fabric formwork is able to receive the application of a liquid-to-solid material (like fiberglass resin, GFRC, concrete, or ice) to create a structural shell. The BA frame utilizes the highly elastic, but predictable, behaviour of the fiberglass to generate anticipated geometries and structural topologies that guide fabric to create an efficient and unique structural shell form. This research explores how the principle stress lines of a shell structure can help to organize the structural topology of the bar placement, allowing the bars to guide the fabric to create a structural form that is congruent with the anticipated force-flow of the shell structure. Because of the liquid state of the structural material applied to the fabric, the BA frame helps to guide the liquid-to-solid material to be concentrated along the PSL of the shell. The opportunity with such a system is that it allows for the design and construction of lightweight shells that perform in efficient ways by organizing structural material where forces are expected, and minimizes it where it is reduced.

Chemical And Mechanical Characterization Of 3D Dental Implants

Presented by: Cristina Fiuza

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Advisor(s): R. França

Co-Author(s): Mohammad Aramfard, Chuang Deng, Rodrigo França

Research Area(s): Mechanics of Materials and Structures, Surfaces and Interfaces

Background. Direct metal laser sintering (DMLS) is a technology that can allow design and manufacture personalized dental implants using (3D) computer model.

Objective: The aim of this study was to compare an experimental DMLS titanium dental implant (Ti6AL4V) (3D) with seven different conventional dental implants (CDI) available on the market.

Methods: All specimens were halved and mounted in epoxy resin, polished and investigated using Nanoindentation. The mechanical tests were performed by Hysitron TI 750 equipment with a Berkovich indenter applying a maximum load of 2000 mN. A minimum of 6 indentations were carried out on each sample and the results were reported as the average of the tests. In addition, the morphological structure of the specimens' surfaces were analyzed by scanning electron microscopy (SEM) and the chemical composition verified by energy dispersive spectroscopy (EDS). All the data were statistically analyzed using ANOVA one-way and Tukey Test.

Results: Chemical composition analyses demonstrated difference between 3D and CDI. Elastic modulus ranged from 72 to 118GPa. 3D values were significantly lower than most of the CDI. The hardness means were for 3D: 4.28 (\pm 0.70) GPa and for CDI the value range was from 4.31 to 5.24GPa with significant scatter among some of them.

Conclusions. DMLS titanium implants have a huge potential for being used in dentistry. The experimental 3D showed to be able to satisfy the chemical and mechanical requirement to be used as oral health procedure.

Effect Of Netrin-1 On The Migration And Chemotaxis Of Human Neutrophils And Breast Cancer Cells In Microfluidic Devices

Presented by: Jolly Hipolito

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Advisor(s): F Lin

Co-Author(s): Hagit Peretz-Soroka

Research Area(s): MEMS/Microfluidic Systems

Jolly Hipolito¹, Hagit Peretz-Soroka¹, Aniel Moya Torres, Ke Yang, Monika Gupta, Markus Meier, Evan Booy, Sean McKenna, Manuel Koch, Jörg Stetefeld, Francis Lin

Netrin-1 is well-known for its chemoattractive and chemorepulsive properties for axon guidance when interacting with cell receptors that include deleted in colorectal cancer (DCC), neogenin and uncoordinated 5 (UNC5). Early reports indicate that leukocytes express UNC5b, inhibiting granulocyte migration and chemotaxis both in vivo and in vitro when interacting with netrin-1. On the other hand, netrin-1 was found to stimulate bi-directional migration of activated T lymphocytes. DCC can also be expressed in various cancer cells, which can mediate a selective advantage for cell survival through its dependence receptor mechanism and can promote tumor invasion. The mechanism underlying netrin-1 mediated immune and cancer cell migration is far from being clearly understood. In this study, we applied a microfluidics approach to quantitatively test the influence of netrin-1 on the migration of purified human blood neutrophils and different human breast cancer cell lines. Our current results showed that netrin-1 decreased the basal motility of purified human blood neutrophils and had a significant effect on neutrophil chemotaxis under different gradient configurations. Furthermore, netrin-1 promoted directional migration of human breast cancer cell lines including MDA-MB-231 and MCF-7 cells. These results will be useful for further investigation of netrin-1 mediated cell migration and the development of relevant therapeutic applications.

Exploration Of Intracellular Proton Currents And Cytoplasmic Streaming (iPC-CS) Model In Driving Amoeboid-Like Motility In A Microfluidic Electrotaxis Assay

Presented by: Hagit Peretz - Soroka

Postdoctoral Fellow at the University of Manitoba, Department of Physics and Astronomy

Advisor(s): FL Lin

Co-Author(s): Hagit Peretz-Soroka, Reuven Tirosh, Jolly Hipolito, Erwin Huebner, Murray Alexander, Jason Fiege, Francis Lin

Research Area(s): MEMS/Microfluidic Systems

Experimental studies showed that actin filaments motion, cytoplasmic streaming and muscle contraction can be reconstituted under actin-activated ATP hydrolysis by soluble nonfilamentous myosin fragments. Thus, biological motility was demonstrated in the absence of a continuous protein network. These results lead to an integrative model for cell motility, which advocates an active role played by intracellular proton currents and cytoplasmic streaming (iPC-CS). In this model, proton and fluid currents develop intracellular electric polarization and pressure gradients, which generate an electro-hydrodynamic mode of amoeboid motion. Under an external electric field (EF), the torque acting on the electric dipole of the cell turns it to move towards the cathode. Such unidirectional energetic proton currents and active streaming are driven by ATP hydrolysis through myosin heads along oriented actin filaments. Key predictions of this model are verified by microscopy visualization and in-depth analysis of purified human neutrophils using microfluidic electrotaxis assays. Three phases in cell motility profiles, morphology, and cytoplasmic streaming are revealed in response to physiological ranges of chemical stimulation and EF application, which are consistently explained by the iPC-CS model. This alternative biophysical mechanism of cell motility provides new insights into bioenergetics and facilitates new biomedical applications.

Poly Vinyl Alcohol Based Humidity Sensing Tag Using Time Gated RCS Measurement

Presented by: Robin Raju

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Advisor(s): G Bridges

Co-Author(s): Bridges, Greg. E

Research Area(s): MEMS/Microfluidic Systems

A radar cross-section based humidity sensing tag is presented. The tag consists of an annular slot antenna loaded with an interdigitated capacitor. The interdigitated capacitor is functionalised using the humidity sensing material PVA . With an increase in humidity, the water content in the polymer elevates, resulting in a change in the dielectric properties of PVA. This change in the dielectric property in turn causes a shift in the resonant frequency and the quality factor of the sensing tag. With a built-in reference and a time gated RCS measurement, it is shown that the change in resonant frequency and the quality factor of the sensing tag can be accurately determined. This approach enables avoidance of both static and dynamic scattering sources. The sensitivity and stability of the tag for various humidity levels were validated through experiments. The bio-compatible design of the tag enables its potential application in non-invasive monitoring of packaged food products for extended shelf life.

Phase Controlled Cavity Magnon Polariton In The Cross Cavity

Presented by: Jinwei Rao

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Advisor(s): C.-M. Hu

Co-Author(s): Jinwei Rao, Yongsheng Gui, Sandeep Kaur, Yutong Zhao, Bimu Yao, Can-Ming Hu

Research Area(s): Photonic and Phononic Interactions

In a microwave cavity, when an electromagnetic wave propagates in a magnetic material, due to the strong light-matter interaction, a cavity magnon polariton (CMP) quasi-particle will be generated. Until now, different methods such as tuning the detune frequency (the difference between the cavity mode and the magnon resonant frequency), adjusting the coupling strength and changing the damping factors have been developed to manipulate the CMP. In this work, we have developed a new technology which can precisely and continuously control the CMP using the phase of the input microwave. We designed a cross cavity which can be viewed as a combination of 2 orthogonal strip-line cavities. By changing the phase difference between the 2 branches, we can continuously alter the polarization of microwave at the center of the cross cavity from elliptical polarization, to linear polarization, and to circular polarization. A low damping bulk ferromagnetic insulator was mounted at the center of the cross cavity so that with the evolution of microwave polarization, the excitation of magnons in the magnetic material can be tuned precisely which allows the control of the CMP. To describe the experimental observations, we put forward a concise classical model, which accurately highlights the key physics of phase correlation between the polarized microwave photon and magnetization dynamics. This phase control of CMP may open up new avenues for materials characterization and microwave applications.

Non-Resonant Radiation Damping In A Coupled Cavity Photon-Magnon System

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Co-Author(s): Jinwei Rao, Bimu Yao, Yongsheng Gui

Research Area(s): Photonic and Phononic Interactions

Non-resonant radiation damping in a planar cavity photon-magnon coupled system is experimentally demonstrated using a planar strip-line cavity along with an YIG sphere. Traditionally, the resonance frequency dispersion and the linewidth exchange due to the cavity photon-magnon coupling has been studied when the resonance frequency of both the modes is matched. In this case, the resonant radiation damping leads to the linewidth exchange between the photon-like and magnon-like hybrid modes. However, the effect of the non-resonant radiation damping, generated due to the magnetic dipole radiation, becomes apparent only when the resonance frequency of the cavity photon-magnon modes is mismatched. At this condition, a careful examination of the change in the linewidth as well as the shift in the magnon resonance frequency reveals the presence of this non-resonance effect. This effect can be explained by using an additional relaxation channel for the hybridized cavity photon-magnon system. This experimental realization and theoretical modeling of the non-resonant radiation damping in cavity photon-magnon systems may help in the design and adaptation of these systems for potential practical applications such as developing long-lifetime multi-mode quantum memories.

An Exploration Of The Spin-Photon Topology

Presented by: Michael Harder

PhD Candidate at the University of Manitoba, Department of Physics and Astronomy

Advisor(s): C.-M. Hu

Co-Author(s): Lihui Bai, Paul Hyde, Can-Ming Hu

Research Area(s): Photonic and Phononic Interactions

Understanding and controlling light-matter interactions is the kernel of materials science and research in this direction has recently revealed the exciting new frontier of strong spin-photon coupling. In systems comprised of ferromagnetic materials and microwave resonators, extremely low damping rates merged with large coherent spin-photon coupling has led to the development of new hybrid quantum information architectures and the realization of coherent spin current control. A key to the success of this new field is an improved understanding of, and the ability to control, both the coupling strength and loss rates. In our recent work we have used a novel and simple technique to systematically control the coupling strength in-situ. Using this capability we have explored the role of damping on the key property of these systems — their excitation spectrum. We find that damping plays a crucial role in the formation of the spin-photon excitations and in particular can lead to the development of certain “exceptional points” in the spectrum. These exceptional points have a topological origin and can be exploited to suppress normal coupling behaviour, as well as to realize interesting mode switching phenomena, which can be tuned by the addition of cavity or spin wave modes. Our spin-photon system therefore shows great promise for the fundamental exploration of exotic physics as well as for novel spintronic applications.

Ferrocene-BOPHY Dyads As Prospective Compounds For Light-Harvesting

Presented by: Dion Nemez

Undergraduate student at the University of Manitoba, Department of Chemistry

Advisor(s): Dr. V. Nemykin

Co-Author(s): Dr. Yuriy V. Zatsikha, Dr. Victor N. Nemykin

Research Area(s): Photonic and Phononic Interactions

BOPHY (bis(difluoroboron)1,2-bis((1H-pyrrol-2-yl)methylene)hydrazine) is a new type of organic fluorophore with distinguished properties such as excellent chemical and photochemical stability, high molar absorption coefficients, and high fluorescence quantum yields. Starting BOPHY molecule was synthesized from pyrrole. Ferrocene containing BOPHY dyads were obtained by Knoevenagel condensation with ferrocenecarboxaldehyde. These compounds have been characterized by NMR, UV-Vis-NIR, as well as X-ray crystallography. Electrochemical and spectroelectrochemical measurements were carried out in order to investigate their redox properties.

Electron-Transfer Processes In Non Covalent Interactions Between Aza-BODIPY Derivatives And Carbon Nanostructures

Presented by: Tanner Blesener

PhD Candidate at the University of Manitoba, Department of Chemistry

Advisor(s): V.N. Nemykin

Co-Author(s): Tanner S. Blesener, Yuriy V. Zatsikha, Gregory T. Rohde, Cole Holstrom, Victor N. Nemykin

Research Area(s): Photonic and Phononic Interactions, Quantum Materials

Boron dipyrromethane (BODIPY) dyes have intense absorption and high quantum yield emission in the NIR region. These characteristics along with their solubility in organic solvents make them popular fluorophores. We have prepared a series of the NIR absorbing aza-BODIPY dyes, which were characterized using NMR, UV-Vis-NIR, fluorescence, HRMS spectroscopy, and X-ray crystallography. Non-Covalent π - π interactions between new pyrene-containing BODIPY derivatives with C60, C70, graphene, and single-walled carbon nanotubes were studied using UV-Vis and steady-state fluorescence spectroscopy. The redox properties of the aza-BODIPYs were investigated using electrochemical and spectroelectrochemical methods. Using x-ray crystallography we were able to study a cocrystallite of our aza-BODIPY molecules with C60.

Dy₂ScNbO₇: A New Spin Ice Candidate?

Presented by: Megan Rutherford

Undergraduate student at the University of Winnipeg, Department of Chemistry

Advisor(s): C Wiebe

Co-Author(s): C. Mauws, S. Haraviford, C. R. Wiebe

Research Area(s): Quantum Materials

Using standard solid state methods, Dy₂ScNbO₇, a member of a new series of pyrochlore oxides was synthesized. While the A-site is occupied by the magnetic Dy³⁺ cation, the B site is split into a mixture of disordered Sc³⁺ and Nb⁵⁺ cations. It appears that Dy₂ScNbO₇ has low temperature spin ice state that is similar to the titanate analogue, Dy₂Ti₂O₇. Attempts to grow single crystals of Dy₂ScNbO₇ have been successful using the floating zone image furnace. Recent characterization results will be presented.

The $\text{Ln}_2\text{ScNbO}_7$ Pyrochlores, Increasing Frustration By Charge Disorder

Presented by: Cole Mauws

MSc Candidate at the University of Manitoba, Department of Chemistry

Advisor(s): C Wiebe

Co-Author(s): C. R. Wiebe

Research Area(s): Quantum Materials

The rare earth pyrochlores of the form $\text{A}_2\text{B}_2\text{O}_7$, are a staple of frustrated magnetism. Due to competing anisotropies and exchange interactions, on a frustrated tetrahedral network, they show a plethora of ground states. One common chemical technique is to substitute 4+ ions (Ti, Zr, Sn, Pt, Ge) on the B-site to alter the magnetism. Here we prepare single crystals of the (5+,3+) charge disordered B-site for A = Pr, Nd, Sm, Gd, Tb, Dy. Preliminary measurements show the magnetism present on the A-site is drastically different than the 4+ analogues

Transport Properties In 1D Integrable Systems

Presented by: Andrew Urichuk

PhD Candidate at the University of Manitoba, Department of Physics and Astronomy

Advisor(s): J Sirker

Co-Author(s):

Research Area(s): Quantum Materials

Low dimension quantum systems have powerful restrictions on their behaviour leading to interesting transport properties like the quantization of electrical conductance in quantum wires, and large heat conductance/ spin diffusion for spin chain materials. By imposing further restrictions on these low dimension quantum systems quantum integrable models appear. Though the number of restrictions necessary to construct a quantum integrable theory might suggest that they are impossible to reproduce in the lab the extreme conditions present in experimental setups for ultra cold quantum gases often result in systems that are nearly quantum integrable. Quantum integrable models have an infinite number of local and quasi-local conserved charges leading to many unique characteristics. Perhaps most notably integrability allows both ballistic and diffusive transport to occur simultaneously, which is understood by identifying some overlap of the quantity with local and quasi-local conserved charges. This overlap is interpreted as meaning that some piece of the non-conserved quantity is protected due to the non-decay of the conserved charge. By exhausting this overlap quantities that survive at long times may be identified and explicitly computed. Recently, a generalized hydrodynamic framework has been developed to the study of quantum integrable systems. Generalized hydrodynamics somewhat mysteriously exhausts this overlap despite it apparently ignoring quasi-local charges, which complicate transfer matrix calculations, altogether. A more complete understanding of the cross-over between integrable and non-integrable quantum systems can be developed by studying the near integrable regime.

Dissipative 1D Open Quantum Systems of Infinite Length

Presented by: Maximilian Kiefer-Emmanouilidis

MSc Candidate at the University of Manitoba, Department of Physics and Astronomy

Advisor(s): J Sirker

Co-Author(s):

Research Area(s): Quantum Materials, High Performance Computing

Experimental realizations of any quantum system involve dissipation, meaning a perfect isolated system becomes an open system. Progress in this field of research is currently driven by numerical renormalization group algorithms such as the time-dependent Density Matrix Renormalisation Group (t-DMRG), and the Time Evolving Block Decimation (TEBD) on finite size systems. Unfortunately, neither method leads to non-equilibrium steady states (NESS), other than the vacuum. In order to address this, we present a renormalization group approach to open one-dimensional quantum systems in the thermodynamic limit. We show that it is possible with our algorithm to reach non-trivial NESS. We conclude that the most accessible ansatz to solve open systems, described by Lindblad master equations (LMS), is a quantum trajectory approach. With our algorithm we analyze an one-dimensional open Bose-Hubbard chain subjected to weak local particle loss in the thermodynamic limit. We time-evolve a Mott insulating Bose-Hubbard ground state and simulate an electron-beam that leads to local particle loss. Our results agree with existing t-DMRG data, however we improved the time the system evolved without boundary effects by a factor 10. This improvement allowed us to obtain the NESS behavior for the density at the dissipative site, the density profiles, and the entanglement entropy. Further, we show that a weak local defect leads to fairly long-ranged correlations. This raises the question whether correlations possibly decay according to a power law in the NESS.

Ultrasound Transport In A Disordered Porous Medium

Presented by: Sébastien Kerhervé

PhD Candidate at the University of Manitoba, Department of Physics and Astronomy

Advisor(s): J.H. Page

Co-Author(s): S.O. Kerhervé, S. Skipetrov and J.H. Page

Research Area(s): Soft and Disordered Materials

Investigating the propagation of multiply-scattered waves in disordered materials allows the characterization of heterogeneous media and may reveal anomalous wave properties. We study wave transport in a porous system consisting of close-packed aluminum beads surrounded by low viscosity silicone oil. In this system, ultrasonic waves undergo many scattering events without significant dissipative losses. The wave transport inside this medium can be modeled by the propagation of two components, the first mainly going through the liquid scattering off the beads and the second traveling through the network of solid beads. Using ultrasonic pulsed transmission experiments, the small ballistic signal at short observation times can be separated from the large multiple scattering coda that extends over a wide range of arrival times. The ballistic signal gives additional information about the fast component going through the liquid and the coda at long times about the slower component going through the solid. The value of kl (wave vector time scattering mean free path), between 4 and 10, obtained for the fast component, suggests that the liquid component can be described using the diffusion approximation ($kl \gg 1$). The measurement of the transverse growth of the acoustic pulse at long times shows that the second, slower, component has to be strongly renormalized (sub-diffusive) or even localized. The results are interpreted by developing a model for the coupled propagation of a diffusive component and a “renormalized” component that is described using the self-consistent theory of localization.

Wicking Properties of Brassica Fiber (Canola Waste Biomass) in Three Different Growth Stages

Presented by: Laura Soriano

Undergraduate student at the University of Manitoba, Department of Biosystems Engineering

Advisor(s): Mashiur, Rahman

Co-Author(s):

Research Area(s): Soft and Disordered Materials

Brassica napus plant (canola biomass) was used as raw material for fibre processing and extraction. An investigation was conducted to determine the wicking behaviour of Brassica napus (B. napus) fibre. The wicking property which is an important comfort property of any textile fibre was studied to assess the B. napus fibre's feasibility for use in textile applications. Wicking is the procedure by which the fibres in a piece of clothing draw sweat away from the skin and up to the surface of the fabric, permitting the dampness to vanish rapidly. A test method was developed to determine the horizontal wicking behavior of single fibre. The wicking property of single fibres was also compared between the different plant growth stages from which the fibre was extracted. The average horizontal wicking rate of B. napus from all stages was found to be 0.184 mm/sec which is much higher than the industry standard (0.08 mm/sec). In addition, the results were compared with cotton, flax and polyester fibres. The horizontal wicking of B. napus fiber was faster than polyester but slower than cotton and flax fibres. These results indicate that B. napus fibre may have potential applications in the textile industry.

Limited Molybdenum Solubility In Borosilicate Glasses? Magnesium To The Rescue.

Presented by: Arun Krishnamurthy

PhD Candidate at the University of Manitoba, Department of Chemistry

Advisor(s): Dr. Kroeker

Co-Author(s): Scott Kroeker

Research Area(s): Soft and Disordered Materials

Borosilicate glasses satisfy most of the requirements for nuclear waste immobilization due to their appropriate physical and chemical properties, as well as their compositional versatility. However, their affinity towards certain fission products is low and can result in compromises to the materials properties if loaded above their threshold limit. For example, molybdenum oxide (MoO_3) has a solubility of ~ 1 wt% in borosilicate glasses. The high cationic field strength of Mo(VI) exerts an ordering effect on the surrounding oxygens atoms which can induce clustering of MoO_4^{2-} units and sequestration of alkali and alkaline-earth ions such as radioactive ^{137}Cs and ^{90}Sr from the glass network into water-soluble crystalline molybdate phases. Since molybdate crystallization is driven by competition amongst cations with different field strength, we have explored the use of high field-strength Mg^{2+} as an additive to preferentially crystallize molybdates into low-solubility, non-radioactive separated phases. We use NMR spectroscopy and x-ray diffraction to study the crystallization behavior of cesium borosilicate model nuclear waste glasses with added Mg to eliminate low-durability alkali molybdate formation. Furthermore, we find that the introduction of magnesium into borosilicate glasses significantly increases the amount of molybdenum that can be incorporated into the glassy network. Multinuclear magnetic resonance is used to gain structural insights to explain these findings and to optimize the compositions for maximum waste loading

Satisfaction with existing clothing labels and need for a clothing safety label: A study based on consumer survey

Presented by: Marjia Khanom

MSc Candidate at the University of Manitoba, Department of Biosystems Engineering

Advisor(s): Dr Rahman

Co-Author(s): Dr. Mashiur Rahman

Research Area(s): Soft and Disordered Materials

This research investigates consumers' willingness to have a new clothing safety label. Unsafe working environments are the main reason for the death and injury for millions of textile and apparel workers in the developing countries. This issue has come to light only after a disastrous accident. It was found that 42% and 26.5% of consumers consider current clothing label 'Useful' or 'Very Useful' and are 'Satisfied' or 'Very Satisfied' respectively among the consumers who are 'Likely' (19.8%) or 'Very Likely' (32.1%) to read the clothing labels. The participants find current clothing labels 'Often' (35.9%) or 'Always' (5.7%) provide enough information while 85% of the participants are 'Interested' or 'Very Interested' to have a new clothing safety label. Further, 84% of the participants consider clothing safety label is 'Important' (41.4%) or 'Very Important' (32.7%). One Way ANOVA revealed that participants over the age of 30 are more likely to read clothing labels than under the age of 30 ($F=12.3$, $df.F1,93$, $p<0.01$). However, non-Canadian consumers find current clothing labels provide enough information over Canadian consumers ($F=4.01$, $df.F1, 93$, $p<0.05$). Pearson Correlation revealed that consumers who are interested in a new safety label do not find the existing clothing labels useful ($r=-0.01$) and are not satisfied ($r=-0.23$). A similar trend observed with the consumers for whom it is important to include a new safety label ($r=-0.04$; $r=-0.22$). The study concludes that consumers want a new clothing safety label that will save millions of workers in the developing countries from deaths and injuries.

BMSCs Laden Injectable Aminodiethoxypropane Modified Alginatechitosan Hydrogel For Hyaline Cartilage Reconstruction

Presented by: Rene Mbeleck

Postdoctoral Fellow at the University of Manitoba, Department of Mechanical Engineering

Advisor(s): Dr Xing, Dr Zhong

Co-Author(s): Mbeleck Rene, Zhong Wen, Xing Malcolm

Research Area(s): Soft and Disordered Materials

Articular cartilage degeneration and defect are caused by aging, joint disease or physical or traumatic injuries. In addition, cartilage has a limited self-regeneration capability due to its avascular and no innervation tissue nature¹. The difficulty in regenerating cartilage is due to the insufficient supply of chondrocytes or the loss of capability to form chondrogenic matrix². To address these concerns, one of the solutions, is the use of bioengineered tissues which can maintain or restore tissue function by replacing the damaged or diseased tissues³. In this work, we used the injectable hydrogels (AALG-CS hydrogels) composed of amino-diethoxypropane modified alginate and chitosan as a tissue-engineering scaffold (chondrogenic differentiation) and as a model for cartilage regeneration. We first introduced an amino-diethoxypropane to the alginate and formed hemiacetal group on it. The hydrogels were formed when the modified alginate met with chitosan. The chemical and rheological properties of the resulting hydrogels were characterized. Then these AALG-CS hydrogels were investigated for chondrogenic differentiation by testing the growth of bone marrow mesenchymal stromal cells (BMSCs) in these hydrogels in vitro. Then for cartilage regeneration, a rabbit cartilage defect was used as model in vivo to investigate if the BMSCs loaded hydrogel could promote the healing process.

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Rheological Study On Bread Dough Properties Using A Power-Law Gel Model

Presented by: Xinyang Sun

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Advisor(s): Martin Scanlon, Filiz Koksel

Co-Author(s): Xinyang Sun, Filiz Koksel, Martin G. Scanlon, Michael T. Nickerson

Research Area(s): Soft and Disordered Materials

The objective of this research was to investigate the interactive effects of wheat cultivar, water content, salt concentration, and mixing time on dough rheological properties using a power-law gel model. The shear storage modulus (G') and loss modulus (G'') of the dough as a function of frequency were modeled in a power-law expression and the mechanical parameters (i.e., S' , S'' , n' and n'') were correlated with dough strength. Doughs prepared from stronger wheat cultivars exhibited a larger S'' , indicating that the strength of the wheat flour dough was significantly affected by wheat cultivar. With increasing water addition, S' and S'' decreased, indicating a softening effect of water on dough. Compared to no-salt doughs, low-salt and high-salt doughs had smaller S' and S'' but larger n'' (i.e., greater change in moduli with frequency). For doughs mixed for various times, an interaction between salt and mixing was observed to affect S' and S'' , indicating that mixing time must be considered when evaluating how dough strength is affected by salt. Compared to optimal- and overmixed doughs, undermixed doughs had smaller S' and S'' , indicating a strengthening effect of mixing on dough. In conclusion, wheat cultivar, water, salt and mixing time exert interactive and individual effects on dough rheological properties. Therefore, ingredients and mixing all need to be considered when preparing bread dough that targets a final product with desirable quality.

Highly Flexible And Resilient Elastin Hybrid Cryogels With Shape Memory, Injectability, Conductivity And Magnetic Responsive Properties

Presented by: Yuqing Liu

Postdoctoral Fellow at the University of Manitoba, Department of Mechanical Engineering

Advisor(s): M Xing

Co-Author(s): Malcolm Xing

Research Area(s): Soft and Disordered Materials, Mechanics of Materials and Structures, Composite Material Systems

Development of conducting or magnetic responsive hydrogels, requires high resilience, flexibility, injectability, responsive sensitivities for the applications of biosensors or bioelectronics. In this work, an ultra-flexible elastin-peptide based hybrid (elastin-gelatin-CNT, EGC) cryogel was fabricated as scaffold to load large amount of rigid functional components, including carbon nanotube (CNT), polypyrrole (PPY) and/or iron oxide magnetic nanoparticles (IONP), for combining excellent conductivity or magnetic responsive property with high elasticity, flexibility, shape memory property and injectable property together. EGC loaded with dispersed PPY aggregates showed highly flexible and injectable property with a moderate conductivity. However, when PPY formed a second rigid network on this soft scaffold, the bicontinuous network exhibited an extraordinarily high resilience enduring 97.5% compressive strain and an outstanding conductivity of 50.1 ± 2.9 S/cm at 90% strain together, as well as excellent bulk pressure sensitive conductivity. Also, the magnetic EGC-IONP-PPY could merge high flexibility, conductivity and magnetic property together, showing the potential as remotely controlled robots or bioactuators.

Skin-Inspired Multifunctional Autonomic-Intrinsic Conductive Self-Healing Hydrogels With Pressure Sensitivity, Ultra-Stretchability And 3D Printability

Presented by: Mohammad Ali Darabi

PhD Candidate at the University of Manitoba, Department of Mechanical Engineering

Advisor(s): Malcolm Xing

Co-Author(s): Mohammad Ali Darabi, Ali Khosrozadeh, Rene Mbeleck, Yuqing Liu, Qiang Chang, Junzi Jiang, Jun Cai, Quan Wang, Malcolm Xing

Research Area(s): Soft and Disordered Materials, Mechanics of Materials and Structures, Composite Material Systems

The advent of conductive self-healing (CSH) hydrogels, a class of novel materials mimicking human skin, can change the trajectory of the industrial process owing to their tremendous prospective of applications in soft robots, biomimetic prostheses and health monitoring systems. Developed herein is a mechanically and electrically self-healing hydrogel based on physically and chemically cross-linked networks. The autonomous intrinsic self-healing of the hydrogel was attained through dynamic ionic interactions between carboxylic groups of poly acrylic acid and ferric ions. A covalent cross-linking is employed to support mechanical structure of the hydrogel. Establishing a fair balance between the chemical and physical crosslinking networks together with the conductive nanostructure of poly pyrrole networks led to a double network hydrogel with bulk conductivity, mechanical and electrical self-healing properties (100% mechanical recovery in 2 min), ultra-stretchability (1500%) and pressure sensitivity. The practical potential of CSH hydrogels was further revealed by their application in human motion detection and their 3D printing performance.

Ultrasonic Microfluidic Actuation With Secondary Bjerknes Forces On Bubbles

Presented by: Maxime Lanoy

Postdoctoral Fellow at the University of Manitoba, Department of Physics and Astronomy

Advisor(s): JH Page

Co-Author(s): Arnaud Tourin, Caroline Derec, Valentin Leroy

Research Area(s): Soft and Disordered Materials, Surfaces and Interfaces, Photonic and Phononic Interactions, MEMS/Microfluidic Systems

In the last decade, the development of microfluidics has motivated the search of new actors that could help handling small objects in laminar flows. Combining various force fields has proved to be a good strategy in classical issues such as particles detection and sorting, drop coalescence, mixing, etc. In the area of physical acoustics, the Bjerknes force, that occurs when an immersed compressible medium undergoes a pressure fluctuation, appears as a potential nominee for microfluidic actuation.

In this poster, we present an original experiment that allows us to follow the trajectory of a free bubble attracted or repelled by a fixed bubble, under the action of an external acoustic field. The role of the frequency of the acoustic excitation and the radii of the bubbles will be discussed in details.

Finally, we tackle a critical configuration and report an evidence of coupling via multiple scattering between both bubbles.

Bubbles In Noodle Dough: Characterization By X-Ray Microtomography

Presented by: Reine-Marie Guillermic

Postdoctoral Fellow at the University of Manitoba, Department of Physics and Astronomy

Advisor(s): J.H. Page, M.G. Scanlon

Co-Author(s): R.-M. Guillermic, F. Koksel, X. Sun, D.W. Hatcher, J.H. Page, M.G. Scanlon

Research Area(s): Soft and Disordered Materials, Complex Natural Systems

Bubbles are found in a huge variety of food products (bread, ice cream, etc...) and are known to bring appreciated texture, mouthfeel and taste. Despite their important role in food properties, the possible presence of bubbles in Asian noodle dough has never been investigated so far. We conducted a series of X-Ray tomography experiments at the Canadian Light Source (Saskatoon, SK) on two types of noodle dough sheets: manufactured with one or ten lamination steps, the dough being rotated 90° between each step. With X-Ray microtomography data, it is possible to detect small bubbles and characterize their size and orientation. We show conclusively for the first time in this study that noodle dough actually contains air inclusions and that the bubble size distribution and volume fraction depend on the manufacturing process (number of laminations). The volume fraction of air entrapped in the dough is higher for the most laminated dough ($\varphi = 1.3$ % for 10 laminations vs $\varphi = 0.9$ % for 1 lamination) while the bubbles are significantly smaller ($\langle r \rangle \sim 20$ μm vs 24 μm), showing that lamination is one of the mechanisms leading to bubble entrapment and break-up. Bubbles are also found to be flat, more concentrated in the center of sheet (in depth), and elongated in the sheeting direction. The characterization of bubbles in noodle dough will be continued with ultrasonic experiments in the near future.

Grain Boundary Structural Phase Transition Under Mechanical Loading In Cu

Presented by: Mohammad Aramfard

MSc Candidate at the University of Manitoba, Department of Mechanical Engineering

Advisor(s): Dr. Deng

Co-Author(s): Chuang Deng

Research Area(s): Surfaces and Interfaces, Crystalline Materials and Nanostructures

Grain boundary structural transition has prominent influence on many properties of polycrystalline materials specially in nanocrystalline metals. While structural and phase transition in multi-component systems is common and phase diagrams are available for many alloy systems, reports on phase transition in single-component systems specially at low dimensions such as grain boundary are rare due to experimental challenges. Phase transformation in grain boundaries and its underlying mechanisms therefore remain unclear and are not well studied until a few recent attempts based on atomistic simulations.

In this talk, we report systematic study on phase transitions of a few types of high-angle symmetric tilt grain boundaries based on molecular dynamics simulations by using Cu as a model system. The focus was to investigate the possible influences of two types of loading, i.e. creep and fatigue, on grain boundary structural transition. One potential application of the grain boundary structural transition on crack healing is also demonstrated, which is facilitated by shear coupled grain boundary motion.

Polyaniline Nanoflowers Grown On Polymer Nanofibers For Flexible Supercapacitors With Prolonged Cyclic Life

Presented by: Ali Khosrozadeh

PhD Candidate at the University of Manitoba, Department of Mechanical Engineering

Advisor(s): M Xing

Co-Author(s): M. Xing

Research Area(s): Surfaces and Interfaces, Surfaces and Interfaces

Polyaniline is a popular pseudocapacitive electrode material that exhibits greater capacitance and energy density than electrical double-layer supercapacitors. However, the brittle nature and poor cyclic stability of polyaniline hinder its practical applications as a freestanding electrode for supercapacitors. It is expected that the stress induced by repeated volume change of polyaniline during cycling is alleviated using polyurethane nanofibers as polyaniline support mimicking mechanical vibration isolators. A flexible electrode for supercapacitors with remarkable cyclic stability is developed by using carbon nanotube-reinforced electrospun polyurethane as a cushiony support for deposition of polyaniline. The in situ polymerization of aniline is controlled such that flower-like polyaniline is grown on individual polyurethane nanofibers resulting in a porous membrane with high surface area and adjustable mass loading of polyaniline by repeating the coating process. In contrast to the continuous degradation of pure polyaniline electrodeposited on carbon cloth, the current design exhibits an excellent capacitance retention of 93% after 10000 cycles of charge-discharge. The cushiony effect of polyurethane and the strong affinity between grown polyaniline and polyurethane nanofibers as well as buffer spaces between nanofibers, which accommodate the volume expansion of polyaniline nanoflowers, all lead to the structural stability of polyaniline during cycling. The facile strategy to attain a stable and flexible polymer electrode could open up new opportunities for flexible and wearable pseudocapacitors.

Electrochemical Reduction Of CO₂ Facilitated By Benzannulated Dihydropyridine Additives

Presented by: Patrick Giesbrecht

MSc Candidate at the University of Manitoba, Department of Chemistry

Advisor(s): D Herbert

Co-Author(s): Patrick K. Giesbrecht; David E. Herbert

Research Area(s): Surfaces and Interfaces

Dihydropyridines (DHPs) have been postulated as active intermediates in the pyridine-mediated electrochemical conversion of CO₂ to methanol; however, the ability of isolated DHPs to facilitate methanol production in a fashion similar to that of their parent aromatic N-heterocycles (ANHs) has not been tested. Here, we use bulk electrolysis to show that 1,2- and 1,4-DHPs (1,2-dihydrophenanthridine and 9,10-dihydroacridine) can mediate the electrochemical reduction of CO₂ to methanol and formate with Faradaic efficiencies similar to those of the corresponding ANHs at Pt electrodes. 1,2-Dihydrophenanthridine furthermore exhibits improved CO₂ reduction activity compared to its parent ANH (phenanthridine) at glassy carbon electrodes. These results provide the first experimental evidence for the participation of DHPs as additives in electrochemical CO₂ reduction.

X-Ray Photoelectron Spectroscopy Characterization Of Three Lithium-Based Glass Ceramics

Presented by: Muna Bebsh

MSc Candidate at the University of Manitoba, Department of Oral Biology

Advisor(s): R França

Co-Author(s): Cristina Fiuza, Rodrigo França

Research Area(s): Surfaces and Interfaces

Objective: A deeper understanding of the mechanical behaviour of dental restoration materials requires an insight into the materials physicochemical composition. The aim of this study was to evaluate and compare the physicochemical composition of three different lithium-based glass ceramics used to fabricate dental restorations at different nanolevel depths of the surface (0 nm, 20 nm, 100 nm). Their bulk compositions were also evaluated.

Method: Three lithium-based glass ceramics: IPS e. max[®] CAD (Ivoclar-Vivadent, Liechtenstein, Schaan), Vita Suprinity[®] (Vita Zahnfabrik, Bad Säckingen, Germany) and Celtra Duo[®] (Dentsply, Hanau-Wolfgang, Germany) were selected in this study (n=6). For the surface analyses a X-ray photoelectron spectroscopy (XPS) was used with a X-ray gun emission set to 15 mA and an X-ray gun anode HT set to 15 kV with power setting 225 W. Laser-Ablation inductively coupled Plasma Mass Spectrometry (LA-ICP- MS) were used for bulk physicochemical composition analysis.

Result: The most significant different between three lithium-based Glass ceramic materials is lithium (Li) concentration, at the surface: IPS e.max[®] CAD 4.9% (± 0.4), Vita Suprinity[®]PC 11.5% (± 0.8) and Celtra Duo[®] 13.7% (± 0.6). However, in the bulk the lithium percentages have increased: IPS e.max[®] CAD 11.4 % (± 3.4), Vita Suprinity[®]PC 17.5% (± 6.9) and Celtra Duo[®] 17.8% (± 8.1).

Conclusion: XPS showed a major difference between bulk and the surface chemical composition for all the tested ceramics.

Keywords: Lithium based ceramics, physicochemical composition

Morphological Study Of Cattail Fiber

Presented by: Koushik Chakma

MSc Candidate at the University of Manitoba, Department of Biosystems Engineering

Advisor(s): M Rahman, N Cicek

Co-Author(s): Dr. Cicek, Dr. Rahman

Research Area(s): Surfaces and Interfaces

An investigation has been conducted to find out the morphological structure of cattail fibre. Bast fiber such as flax, hemp and jute are extracted from the outer layer (Epidermis) of the plants. As a result, the yield (%) of these fibers ranges between 10 to 20% only, whereas current research on cattail plant was found that when treating in alkaline solutions, whole cattail plant transformed into fiber and the yield (%) of cattail fiber was found to be as high as 40 to 60% depending on the extraction temperature and time.

The scanning electron microscopy (SEM) micrography reveal that the cattail fibers lie inside the epidermis layer. The areas of the plant and fiber sections was found to be 38.5 mm^2 and 20.1 mm^2 respectively and the ratio of fiber to plant area is 52.0% which is within the range of fiber yield (%). It appears that each fiber comprised of numerous cells (≈ 55 in $740 \text{ }\mu\text{m}^2$, $4.5 - 6.0 \text{ }\mu\text{m}^2/\text{cell}$) which are elliptical in shape and the distance between each cell is about $0.70 \text{ }\mu\text{m}$. Each cell has lumen and the size of the lumen varies which was as high as $1.03 \text{ }\mu\text{m}$. From the morphological studies, it is concluded that the cattail fiber could be used for both textile and biomedical applications.

SHArK North: Investigation Of Metal Oxides As Water Oxidation Catalysts

Presented by: SHArK North

Daniel McIntyre Collegiate Institute and Grant Park High School

Advisor(s):

Co-Author(s): Gyeongwon Lee, Renmar Palma, Kurt San Jose, Nicolas Pausing, Nicklaus Maligaya

Research Area(s): Surfaces and Interfaces, Composite Material Systems

SHArK North is an outreach program here at the University of Manitoba, in association with CCI Solar, where high-school students (from DMCI and Grant Park) develop research skills and explore new photoelectrode materials for artificial photosynthesis. In particular, students investigate the application of ternary mixed metal oxides as photoelectrodes for water oxidation, selecting from a host of light absorbing, structural and charge compensating metal salts. This work presents the findings of the 2016-2017 SHArK North team, with an iron-molybdenum-barium mixture providing the best activity towards water oxidation out of the mixtures tested.

Impact of SiCl₄ Precursor Flow Rate On Growth Rates And Doping Of VLS-Grown Microwires

Presented by: Sridhar Majety

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Research Area(s): Surfaces and Interfaces, Crystalline Materials and Nanostructures

Silicon microwires fabricated using bottom-up vapor-liquid-solid process are critical component for solar fuels generation. The influence of SiCl₄ flow rate on the growth rate, doping, resistivity and morphology of microwires has been investigated. The growth rate, microwire resistivity and doping concentrations are studied at different flow rates of SiCl₄ (10 sccm, 5 sccm, 3 sccm, 1 sccm). Scanning electron microscopy was used to study the sidewall facet morphology of the microwires. The growth rate variations are in agreement with the observations of Shepherd et al., ranging from 7.5 μm/min at 10 sccm to 0.15 μm/min at 1 sccm. Electrical, two-point probe measurements, using a direct-contact technique involving tungsten probes controlled by piezo actuated micromanipulators, formed ohmic contacts with the microwires. The doping concentrations show an exponential dependence on the flow rate. It was verified that the sidewall morphology changes when the flow rate of SiCl₄ is changed during growth. The number of sidewall facets changes from 12 to 6 facet when the flow rate is shifted from 10 sccm to 1 sccm and reverts to 12, when SiCl₄ flow rate revert back to 10 sccm. These transitions were observed during growth of a single wire. The density of the fine band morphologies observed on the sidewalls increases with decreasing the flow rates. This is attributed to the increased influence of fluctuations in the SiCl₄ flow rate as it is decreased.