Complexation of α-Tocopherol and Quercetin with α-, β-, and γ-Cyclodextrins

Wade Alexander, John Koontz, Joe Marcy

Antioxidants used in the food industry to extend shelf life are added to food products in a single dose. Controlled release from food packaging is desired to limit the addition of antioxidants in high concentrations. Controlled release can be achieved using inclusion complexes of antioxidants and cyclodextrins. This study examines complexes of α-tocopherol and quercetin with α-, β-, and γ-cyclodextrins using ^{1}H NMR titrations and FT-IR spectroscopy. It was determined that solution NMR does not provide enough information to prove inclusion of practically water insoluble compounds. Solid-state FT-IR techniques also proved inconclusive in proving inclusion.

KEYWORDS: Cyclodextrins; antioxidants; inclusion complexes

A support free method of isolating trimetallic nitride endohedral metallofullerenes

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ABSTRACT

Since the inception of fullerene science, the isolation of particular fullerenes from others has been a substantial problem and has hindered the study of these materials. With the budding of research regarding trimetallic nitride template endohedral metallofullerenes (TNTs) and their myriad potential applications, the development of a means to quickly and inexpensively obtain pure samples of a variety of TNTs is necessary. Herein described is a method of separation which involves the selective solid-liquid state reaction of 9-methylanthracene with soot extract and generates a Diels-Alder adduct with empty cage fullerenes that is soluble in ether. Preliminary results show that the adducts can therefore be removed from the desired TNT by solvent separation, resulting in a method of purifying TNTs that is inexpensive, time effective follows the practices of green chemistry.

Simple Fractionation of Hyperbranched Polymers

Eric Armstrong, Min Mao, Dr. S. R. Turner

ABSTRACT

Two methods were devised for the simple fractionation of the polyesteramide Hybrane S 1200 and the carboxylic acid terminated aromatic hyperbranched polyester poly 5-(2-hydroxyethoxy) isophthalic acid. The method for Hybrane proved to be more extraction based, as its dissolution in dichloromethane followed by the introduction of hexane cause a bilayer to form, which was subsequently separated at the end of each trial. It was observed that though the additions of hexane decreased in volume while the volume of dichloromethane was kept virtually constant, the clear top hexane layer grew in relation to the bottom dichloromethane one with each successive trial. On the other hand, the method for the hyperbranched polyester consisted of continually greater percentages of diethyl ether being added to THF, in which poly 5-(2-hydroxyethoxy) isophthalic acid was dissolved. Precipitates collected from 10 %, 20%, and 25 % v/v ratios of diethyl ether to THF yielded polydispersities of 1.65, 2.08, and 1.94, respectively. In addition, a new method was proposed for the synthesis of methyl 3,5 di(2-hydroxyethoxy) benzoate monomer from 3,5-dihydroxy benzoate, which, if successful, could provide means for the synthesis of another carboxylic acid terminated aromatic hyperbranched polyester on which simple fractionation can be tested.

Synthesis and Characterization of Magnetic Polylactide Nanospheres

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ABSTRACT

Poly(D,L-lactide) stabilized magnetite is a biodegradable, biodispersable complex that can be further incorporated into nanospheres. Subsequently, these nanospheres can be used for biomedical applications such as targeted drug delivery and biospecific cell separation. Poly(D,L-lactide) was synthesized using a trivinylpropoxysilane to polymerize a 20,000 g/mol homopolymer. The terminal vinyl groups on the poly(D,L-lactide) homopolymer were further functionalized with carboxylic acid groups by adding mercaptoacetic acid across the pendent double bonds in an ene-thiol free radical reaction. The carboxylic acid groups are designed to bind to the surface of magnetite with different weight percentages of magnetite while the poly(D,L-lactide) provide dispersion stabilization in polylactide solvents. Subsequent nanosphere formation of these complexes ranged in size from 110nm-130nm as indicated by SEM.

Synthesis and Characterization of Hydrogen Bonding Polymers and Blends with Phosphonium Salts

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ABSTRACT

The effect of introducing both hydrogen bonding and ionic characteristics into a hydrogen bonding block copolymer by blending it with a trioctylphosphonium uracil salt was studied. An adenine containing triblock copolymer was synthesized using nitroxide mediated stable free radical polymerization. A novel trioctylphosphonium uracil salt, which is compatible with the adenine block copolymer due to hydrogen bonding interactions, was synthesized. The hydrogen bonded blend of the adenine triblock copolymer and trioctylphosphonium uracil salt was characterized using AFM, DSC, solution rheology, and DMA. The hydrogen bonding interactions of a phosphonium salt with a block copolymer in both solution and solid state were demonstrated. In addition to the synthesis of a trioctylphosphonium uracil salt, a novel, water-soluble adenine triphenylphosphonium salt was synthesized.

The Influence of Oxidative Stress on Immune Response in Chickens

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Virginia Tech Summer Undergraduate Research Program

Abstract Oxidative Stress (OS) occurs when an organism has higher levels of oxidants than antioxidants. In this research, OS and Immune Response (IR) are analyzed in chickens. We are evaluating OS and IR to determine if a higher oxidative state would induce a higher or lower immune response in the birds.

Key words: Malondialdehyde, Thiobarbiturate acid reacting substance, White leghorn chicken, oxidative stress, immune response

MODELING OF AN IONOMER ACTIVE FLUID MIXER

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August 2006

Abstract

Mixing fluids at small scales is difficult due to dominant viscous forces. Active mixers increase mixing by stirring the fluid and are tuneable and controllable by varying the input signal. Ionomers represent a novel and inexpensive active mixing technology. In this paper, preliminary calculations are presented on the effectiveness of an ionomer mixer. Current ionomer performance levels are examined and a target performance level is also presented. Numerical simulations are also performed with different geometries. Order of magnitude calculations and numerical simulations show that ionomers can be used to increase mixing significantly.

Preparation of Cellulose Nanocrystal Solid Films

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ABSTRACT

Suspensions of cellulose nanocrystals produce optically active films when dried. The films optical properties are due to the formation of a chiral nematic liquid crystalline phase. All suspensions produced by acid hydrolysis using 64%wt sulfuric acid in a ratio of 8.75 mL of acid to 1 g of cellulose formed the chiral nematic phase. We have examined the effects on the formation of the chiral nematic phase by: drying films in a 7 T magnetic field, varying hydrolysis times, and desulfonation of the cellulose nanocrystals. Drying in a 7 T magnetic field aligned the helix parallel to the applied magnetic field, producing more uniform distribution of the chiral nematic order and, therefore, more colorful film. The modification of hydrolysis times produced suspensions of varying degrees of sulfonation. The desulfonation of the cellulose nanocrystals also produced suspension with a range of degree of suflonation. Suspensions consisting of nanocrystals with lower degrees of sulfonation produced more colorful films. The degree of sulfonation appears to directly influence the optical properties of the solid films.

The Development of Compression Moldable Laminate Bipolar Plates for Application in Fuel Cells

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ABSTRACT

Graphite and polymer composite laminate bipolar plates were compression molded with the intention of developing a highly producible bipolar plate for application in polymer electrolyte membrane fuel cells (PEMFCs). The electrical conductivity and mechanical strength properties were analyzed as well as the affects of production techniques on physical properties and fuel gas flow channel formation. The plates consisted of a wet-lay paper core layer and two laminate layers on either side of the core layer. Plates were produced by a 1-step process, simultaneous compression of all layers, and a 2-step process, pre-consolidation of wet-lay material with later addition of laminate layers. Electrical conductivity was found to be improved by increasing graphite concentrations, increasing laminate layer volume, and using the 1-step method as apposed to the 2-step method. Small changes in laminate layer volume were found to have little impact on mechanical strength. Although the 1-step method was found to provide better electrical and mechanical properties, the 2-step method may result in a more applicable form of large scale production.

Characterization of Optical Properties and Swelling Behavior in Thin Films of Biphenyl Poly(Arylene Ether Sulfone) Copolymers

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Abstract

Fuel cells are quickly becoming a promising solution as alternatives for fossil fuels and may potentially be used for technological applications ranging from electronics to automobiles. The dielectric constants and refractive indices of biphenyl poly(arylene ether sulfone) copolymers with 35 mol% sulfonation in the salt form (BPS-35) and acid form (BPSH-35) confined to thin films were investigated. Furthermore, the swelling behavior of BPS-35 and BPSH-35 thin films in common organic solvents was also studied. Multiple incident media ellipsometry (MIM) was used to characterize the polymers' optical properties as well as their swelling behavior. The dielectric constant and refractive index of BPS-35 were determined to be 2.61 ± 0.07 and 1.62 ± 0.02, respectively. BPSH-35 polymer was found to have a dielectric constant of 2.72 ± 0.04 and a refractive index of 1.64 ± 0.01. The films used in this study were too thin for accurate detection of swelling because the changes in ellipticity of these films arising from swelling are comparable to the error associated with MIM ellipsometry measurements. However, deviations in the values of dielectric constants, refractive indices, and thicknesses for BPS-35 and BPSH-35 films obtained from MIM ellipsometry measurements using acetone, ispropanol, ethanol, and methanol as the second media were consistent with the film swelling in these media.

Hydroxypropyltrimethylammonium-Xylan Adsorption Studies onto Model Surfaces via Surface Plasmon Resonance Spectroscopy

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Abstract

Hemicelluloses play an important role during cell wall biogenesis by binding crystalline cellulose-rich and amorphous lignin-rich domains at the interface. In this study, the self-assembly of hydroxypropyltrimethylammonium-xylan on model surfaces is probed by surface plasmon resonance (SPR). Four model surfaces on gold: regenerated cellulose, and methyl, hydroxyl, and carboxylic acid terminated self-assembled monolayers (SAMs) provide insight into intermolecular interactions driving hemicellulose self-assembly onto cellulose. The observations of comparable adsorption onto cellulose, and the methyl and carboxylic acid terminated SAMs, along with weak adsorption onto the hydroxyl terminated SAM yield the surprising conclusion that hydrophobic interactions are at least as important as electrostatic interactions for driving self-assembly, and that hydrogen bonding plays a minor role.

Chemical Composition and Sequence Length Effects on Proton Exchange Membrane Transport Properties

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Proton exchange membranes are an integral part of fuel cells, which impact performance, stability, and applicability. Hydrophobic-hydrophilic poly(perfluoronated arylene ether – disulfonated arylene ether sulfone) BisSF-BPSH multiblock copolymers were synthesized for use as proton exchange membranes. Membrane morphology was investigated as a function of chemical composition and block length. The effect of sequence length on the morphology provided a structure-property relationship for understanding proton transport mechanisms. Proton conductivity, hydration numbers, and the self-diffusion coefficient of water were studied to establish the properties of this copolymer series, Nafion, and a random copolymer, BPSH-35. Under partially hydrated conditions the block copolymers exhibited superior behavior compared to random copolymers due to enhanced nanophase separated morphology. The BisSF-BPSH series surpassed the performance of Nafion at all temperature under fully hydrated conditions. Activation energy for proton transport decreased with increasing hydrophilic fraction sequence lengths at longer block lengths. Proton conductivity and the water self-diffusion coefficient increased with increasing block lengths. The self-diffusion coefficient of water dominated proton transport under partially hydrated conditions. Water uptake and the hydration number decreased with an increase in the hydrophobic fraction sequence length for a given ion exchange capacity. The selectivity of the membranes increased at longer block lengths with larger hydrophobic fractions.

Solid-Phase Synthesis of a Potential Pin1 Inhibitor

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ABSTRACT

The peptidyl propyl cis/trans isomerase (Pin1) is a small, primarily nuclear, protein that is an essential component in the regulation of cell division. Research has shown that Pin1 is over produced in various types of cancerous cells. Inhibition of Pin1 activity could halt cellular division and therefore cause the initiation of apoptosis in cancerous cells. We are interested in the design of a potential non-competitive inhibitor of Pin1, Val-Pro-Arg-pThr-Pro-Val, using solid-phase synthesis with an Fmoc protection strategy. The resulting yields from several trials lead to subtle changes in the synthesis procedure that will result in more substantial yields of this peptide in future synthesis. This peptide sequence was chosen based on its binding preference for the WW domain over the catalytic site of Pin1. If the designed peptide demonstrates non-competitive inhibition, then the option for cancerous cells to adapt to the inhibitor could be virtually eliminated. The final inhibitor will be tested to determine its IC_{50} and K_i values to help determine its effectiveness for inhibiting Pin1 activity and its potential value in developing a new drug strategy against cancerous cells.

Carbon Nanowire Based Biological Fuel Cell Anode Design with the Utilization of *Nitrosomonas europaea*

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Target Journal: *Biotechnology and Bioengineering*

Abstract

The feasibility of a new anode design for a biological fuel cell (or biofuel cell) involving the use of carbon nanowires was investigated. A preliminary study examined its average power production and usage lifetime. We used the metabolic process of *Nitrosomonas europaea*, which convert ammonia into nitrite thereby releasing two electrons. This bacterium is commonly found in wastewater treatment plants and used for ammonia conversion. Previous experiments with biofuel cells have used electron mediators to carry electrons from the surface of the bacteria cells to the anode. We hypothesize that by growing carbon nanowires on the surface of an anode it is possible to develop a biofilm on its surface. This biofilm, that contains bacteria, should allow direct electron transfer from the cell surfaces to the anode, thus increasing power production and reliability. Carbon nanowires were directly grown on a stainless steel wire mesh anode using the flame synthesis method. The nanostructure growth involved a specific exposure time of the stainless steel substrate to a well-defined steady flame. Parametric investigations were performed to characterize the optimal height at which the substrate would have to be placed in the flame above the burner rim, and the air and ethylene flow rates used to establish the nonpremixed flame in order to maximize the nanowire yield on the anode. Thereafter, the biofuel cell was run over a three day period. Since the fuel cell design involves a batch and not a continuous supply of bacteria and ammonia, power production ceased after roughly 35 hours. Over this time period the average biofuel cell power production was 20 $\mu W/cm^2$ of anode. While previous biofuel cell designs using electron mediators have produced power up to 78.7 $\mu W/cm^2$ of anode, we are hopeful that further work, particularly involving continuous bacteria and ammonia supply, will enable our design's practical use in a wastewater treatment plant.

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Determination of MEA Material Properties usine 3D Digital Image Correlation System

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ABSTRACT

There are many benefits to fuel cells that make research and development a very pressing matter. Obtaining material properties of the membrane electrode assembly (MEA) is a significant part of Proton Exchange Membrane fuel cell (PEMFC) research. This enables understanding of how the membrane will act while in use in the fuel cell. The desired values of this research were simple blister and tensile tests. The behavior of the MEA blister and tensile tests were characterized using ARAMIS optical measurement system (GE Optical Measuring Techniques, Braunschweig, Germany). This technique relies on a 3D digital image correlation system (DIC) to determine the deformations and strains throughout the experiment. It is a valuable technique of non-contact evaluation. From this method, an apparent Elastic Modulus and Poisson's ratio was found to vary with pressure throughout the blister. A more concrete Poisson's ratio value of 0.3995 was obtained from the simple tensile test. The results demonstrated that the DIC is an advantageous tool in fuel cell research.

Comparison of Electrocatalysts and Membrane Materials (BPSH-35 and Nafion® 117) for Direct Ethanol Fuel Cells

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Abstract

A direct ethanol fuel cell (DEFC) is a proton-exchange membrane fuel cell (PEM-FC) that uses the widely available plant-based ethanol as a fuel directly oxidized on the cell electrode. DEFCs do not require additional processing of a raw fuel and the fuel has a much higher energy density than H_2 gas, both of which tremendously decrease the cost, size, and complexity of the supporting system for a DEFC. These benefits give the DEFC a large potential for commercial application such as anywhere from portable laptop power to transportation to micro fuel cells. Much of the research insight developed for the more popular direct methanol fuel cell (DMFC) can be cross-applied to the DEFC due to similar alcohol chemistry of the fuels.

Molecular Docking and Monoamine Oxidase B:
A Computational Approach to Novel Inhibitor Discovery

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ABSTRACT

Monoamine oxidase B (MAO-B) functions in the oxidative deamination of neurotransmitters with a preference for phenylethylamine and benzylamine. MAO-B inhibitors have anti-parkinsonian effects as well as other neuroprotective properties. Our efforts focused on molecular docking to this enzyme using UCSF's DOCK software, in search of novel inhibitors. We first provide validation for our docking methods, demonstrating the docked positions are accurate with respect to known crystal structure positions. We then dock a group of covalent inhibitors to aid in a mechanistic study of the enzyme. Finally, we dock a group of potential noncovalent inhibitors obtained from the ZINC database. We also examine potential problems with the active site conformation variations and DOCK energy scores.

Viscoelastic Properties of Poly(dimethylsiloxane) and Octaisobutyl-POSS Blends

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Polyhedral oligomeric silsesquioxanes (POSS) have been an active area of research for more than twenty years. Applications of POSS include high-temperature systems and space-survivable coatings. In this study, the viscoelastic properties of nonamphiphilic octaisobutyl-POSS and amphiphilic poly(dimethylsiloxane) (PDMS) blends at the air/water interface were studied as a function of POSS composition. In surface pressure-area isotherm studies, the isotherms resembled PDMS although the collapse pressure of the monolayer decreased with increasing octaisobutyl-POSS content. Surface light scattering (SLS) studies of capillary waves revealed that increasing the percentage of POSS in the blends did not significantly alter the dilutional viscoelastic properties of the film. In this respect, octaisobutyl-POSS can be regarded as a true filler whose only role at the air/water interface is to confine PDMS to a smaller effective trough area.

The Effect of Particle Size on Alumina - Fluorine Interactions during MEA Combustion in a Microwave Field

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Abstract

The purpose of this study was to determine if alumina (Al_2O_3) would undergo significant physical/chemical changes in the presence of fluorine during membrane electrode assembly (MEA) combustion in a microwave (MW) field. This project investigated three different particle sizes of Al_2O_3 which were directly exposed to fluorine as a result of MEA combustion. The results of these experiments showed that MEAs may be combusted in a MW field and that fluorine will react/bond with Al_2O_3 without consuming the Al_2O_3. In addition, the data suggests that the surface area, not the particle size, dictated the amount of Al_2O_3 - fluorine interaction.

Keywords

Membrane Electrode Assembly (MEA), Alumina, Fluorine, X-Ray Photoelectron Spectroscopy (XPS), Fourier Transform Infrared Spectroscopy (FTIR), Microwaves (MW)

Characterization of Ionic Polymer Membranes for Application as a Heart Sensor

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ABSTRACT

The purpose of this study was to characterize ionic polymer membranes for use as an electromechanical sensor, specifically as a sensor to monitor mitral valve prolapse. The membrane used in the experiment was plated with four layers of platinum and gold electrodes, and then exchanged to one of four different ions: lithium, cesium, *tert* butyl ammonium and 1-ethyl-3-methylimidazolium. Each ion-exchanged membrane was tested for its electromechanical sensing abilities using a linear actuator to cause displacement and a software program to measure electrical charge. Cesium proved to have the greatest range of current response, and also continued to operate well at higher frequencies. Lithium gave the quickest response to displacement, but had a smaller current response range and lost ability to respond well at higher frequencies. *Tert* butyl amine gave a very poor response, and 1-ethyl-3-methylimidazolium gave no consistent results. The membrane was further tested by placing lithium-exchanged membranes into various solutions for one hour and then characterizing their response. It was found the solutions greatly damage the membrane's ability to respond.

Organic Solar Cells Using Ionic Self Assembled Multilayers

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I. Abstract

The object of this research was to test the photovoltaic properties of a bilayer composition of alternating thin films of two different organic materials, Alcian Blue (AB), an electron donor and Polyaniline Sulfonic Acid (PASA), and electron acceptor. These material have a band gap of the order of visible light. Hence, it was hoped that when light was incident on a film composed of these materials, photo-excitation, followed by charge transfer, would occur from AB to PASA and the electrons would be collected at aluminum electrodes as photocurrents. Had the materials worked well together, it would have demonstrated a new approach in the construction of Organic Solar Cells. By using the Ionic Self-Assembled Multilayers (ISAM) procedure, these two materials were deposited on top of each other, in a succession of alternating layers, the substrate being a specially prepared glass slide. These layers naturally diffused into each other, creating a connected path between the layers of each material and allowing for charge transport throughout the entire device. To test the photovoltaic properties of these devices, the I-V characteristics under monochromatic illumination, where light of a specific wavelength was made to shine on them while current was measured for different applied voltages. The power outputted by the device was calculated by multiplying the current with the voltage and the maximum power thus obtained, could be compared with the power of the lamp to determine the overall efficiency of the device. The efficiencies of AB and PASA together were compared with the efficiencies produced by combinations of inert, non-photovoltaic materials, AB and PAA together and PAH and PASA together. As it turned out, the efficiencies of AB and PASA together were no better than the efficiencies of either combined with an inert material, and these efficiencies were much too low to be used in any practical energy applications.

Quantitation of Oxidative DNA Damage of Peripheral White Blood Cells and Cells Grown in Culture

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ABSTRACT

Oxidative tissue damage can result from an overproduction of reactive oxidant species (ROS) during the persistence of disease states such as obesity, cancer, atherosclerosis, and diabetes. Damage from these ROS extends to the macromolecules within the cells of these tissues, particularly lipids, proteins, and DNA. Assays have been developed to measure numerous biomarkers within each of these classes. DNA oxidation can be monitored by measuring 8-oxoguanine (8-oxoG) levels in cells experiencing high oxidative stress conditions. Guanine residues are susceptible to ROS, and quantitation of 8-oxoG has been made simple by the development of convenient and reliable assays that have replaced more complex measurement methods such as HPLC. The purpose of the study presented here is to evaluate the utility of an assay designed for measuring 8-oxoG levels in a human system when applied to isolated feline white blood cells and human breast cancer cells grown in culture. In both of these systems, cells experience high oxidative stress resulting from obesity in the feline model and cancer cell proliferation in the *in-vitro* model. Effects of antioxidant-enriched reagents on both of these systems are measured by assaying for 8-oxoG.

Twenty adult, obese cats were fed an antioxidant-enriched diet for controlled acute weight loss over a 6-week period. Data indicate a decrease in fat mass concomitant with reduction in 8-oxoG levels, which suggests a decrease in oxidative stress. Subjects receiving a diet containing less antioxidant experienced an increase in fat mass along with an increase in 8-oxoG levels.

Two human breast tumor cell lines (T-47D, ER+; MDA-MB-231, ER-) were treated with two forms and two doses of pomegranate juice. In all cases, 8-oxoG levels decreased dramatically compared to untreated cells. Decreased proliferation and metabolic activity were observed with increasing dose, which appears to correlate with the decrease in oxidative conditions.

The Synthesis of Silver Nanocubes for Surface Plasmon Effects

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ABSTRACT

Silver nanocubes have been shown to enhance surface plasmon characteristics, which can be employed in various research applications. The Xia group's research at the University of Washington found that a basic polyol reduction method and two variations of an etching process involving iron and hydrochloric acid produced nanocubes. The basic polyol reduction method used high concentrations of silver nitrate (0.25M) and polyvinylpyrrolidone (0.375M) in ethylene glycol (EG). These solutions were injected into a bath of pure EG and reacted for 45 minutes. This, as well as all other products, underwent thorough analysis via absorbance, dynamic light scattering, zeta potential, and scanning electron microscopy. Few sharp-edged particles were found using this method as either quasi-spherical or irregularly shaped particles comprised the majority of the product. The other procedures involved the concept of etching, where the dissociation of one type of product (nanowires) can promote the formation of another product (nanocubes). The etching process typically required 44 hours to complete [1], but with the addition of hydrochloric acid, or iron and sodium chloride, the reaction time was greatly reduced. For the iron-controlled etching process, small traces of iron (0.44 μM iron(II) acetylacetonate or 0.44 μM iron(III) acetylacetonate) and sodium chloride (0.06 mM) were added to a 144 mM solution of polyvinylpyrollidone (PVP) dissolved in EG. This reacted with a 94 mM solution of silver nitrate in ethylene glycol over 15 hours. Numerous sharp-edged triangular plates were synthesized, and nanowires were either reduced to nanorods or produced in significant number depending upon the concentration of iron used. The hydrochloric acid alternative of the etching process required similar concentrations of silver nitrate and PVP solutions in glycol (94 mM and 147 mM, respectively) as the iron process. A small addition of 3 mM hydrochloric acid in glycol to the pure EG bath preceded the injection of the solutions. A reaction time of 24 hours took place, detailed by numerous color changes. Several cubes were found, but the resulting product was mainly wires. By exploring the three general procedures proposed by the Xia group, syntheses were carried out by the Davis lab to produce silver nanocubes. Though nanocubes were not produced in high yield, the results give evidence that future experiments could be used to achieve this goal.

Reconstruction of 3D Porous Microstructure of the Cathode Catalyst Layer of a PEM Fuel Cell

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ABSTRACT

Computational modeling of PEM fuel cell is an important tool in understanding the different electrochemical reactions and transport phenomena occurring in PEMFC so as to develop more efficient PEM fuel cells. Cathode catalyst layer plays an important role in a PEM fuel cell because of the electrochemical reactions occurring in this layer. Proper modeling of the catalyst layer is required if an accurate prediction of the cell behavior is desired. This paper tries to approach the modeling of the catalyst layer in a different way as compared to previous approaches which model the active catalyst layer as an infinitely thin interface or as macro-homogeneous porous layers. The key idea is to model the actual porous microstructure of the cathode catalyst layer. Several different methods can be used to reconstruct the porous geometry but using 2D microscopic images to obtain 3D geometry with stochastic models is one of the cost efficient and a relatively easier method. This paper explains the 3D reconstruction of the catalyst layer from the 2D scanning electron microscope (SEM) images using granulometry law method.

Supramolecular Structures Containing a Synergy of Hydrogen Bonding and Photo-crosslinkable Sites

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Abstract:

Hot melt pressure sensitive adhesives solidify and adhere upon cooling and a slight application of pressure. These types of adhesives have many positive characteristics. They are solvent free and cheap. Hot melt adhesives eliminate the hazardous air pollutants found in organic adhesives. Another major advantage to this type of adhesive involves the ability to tailor their composition to meet desired characteristics and requirements. Compounds such as acrylics and photo-reactive groups have been added to pressure sensitive adhesives to change the properties and produce more efficient adhesives. Urethane groups and cinnamate groups are examples of compounds being added to hot melt adhesives.

The objective of our research was to investigate how associations influence the photo-reactivity of macromolecular architectures. More specifically, we wanted to examine how the hydrogen bonding of urethane groups influenced the rate and efficiency of the photo-reactivity of cinnamate groups in low T_g acrylics. A precursor copolymer compound of n-butyl acrylate-*co*-hydroxyethyl methacrylate was functionalized with hydrogen bonding urethane groups and photo-curable cinnamate groups at various relative mole percentages. The effects of the hydrogen bonds on the cinnamate curability were examined through thin film UV-vis spectroscopy and UV-rheology. The thin film spectroscopy showed that in thin films, the adhesives containing the most urethane and the least amount of cinnamate had the fasted curing time. As the amount of urethane in the sample increased, the curing rate also increased. The UV-rheology showed that as the amount of cinnamate increased in the samples, the difference in starting and ending viscosities increased.

Electrochromic Properties of Thin Conductive Poly (aniline 2-sulfonic) acid (PASA) Films, Formed by Ionically Self-Assembled Monolayers (ISAM) Technique

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Department of Physics Virginia Polytechnic Institute and State University
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Abstract

A new electrochromic device (ECD) designed and constructed base on Poly (aniline 2-sulfonic) acid, (PASA), as active electrochromic polyanion, and Poly (allylamine hydochloride), (PAH), as inactive polycation, was proposed and studied in this work. Cyclic voltammetry (CV) technique was employed to study redox properties of the device and to help to determine the operating voltage of the device. It was determined that the PAH/PASA ECD has two redox states between -1.0V and +1.0V. The ECD with 40 bilayers demonstrated dark green to light brown to dark gray electrochromism, in -1.0V to +1.0V window. The major transmittance occurred at -0.8V (dark green) and +0.8V (dark gray), The ECD in relax state, no voltage applied, is light brown. At -0.8V, in visible spectrum, the highest contrast ($\Delta T = 27\%$) appeared at ~690nm (dark green) and at +0.8V the highest transmittance in visible range was a broad range between ~600 to ~710 nm.

Analysis of Dissolved Oxygen

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ABSTRACT

Dissolved oxygen (DO) measurements have become increasingly important as the applications for DO levels have expanded. Several DO detecting instruments exist in the market today; however, each DO method has its own specifications and operation principles. The differences among the probes require users to distinguish between the capabilities and performance of individual probes. The objective of the current research is to evaluate and compare DO detecting instruments. The two probes chosen for this study were the Mettler Toledo 4000e oxygen probe and the Foxy Fiber Optic Ocean oxygen sensor. The instruments were compared based on various design elements such as power source, user friendliness, portability, life span, theory of operation accuracy and performance under various experimental conditions. We chose antioxidants to demonstrate the methods and techniques of the probes aforementioned because previous research shows a decreasing trend in DO levels with the presence of an antioxidant. The specific antioxidants chosen for this study were L-Ascorbic acid as a commercial source antioxidant and apple juice as a natural source of antioxidants. The overall performance and accuracy of the Mettler Toledo oxygen probe proved superior to that of the Ocean Optics.

Prevalence of Obesity and Its Relationships to Hyperinsulinemia and Oxidative Stress/Inflammation in Horses

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ABSTRACT

Obesity is a major health problem in humans due to its association with insulin resistance (IR), diabetes mellitus, and cardiovascular diseases. Anecdotal evidence suggests that equine obesity is also a growing problem because obese horses may be predisposed to IR, oxidative stress/inflammation, and its co-morbidities such as laminitis. It has been estimated in a study conducted by the United States Department of Agriculture (USDA) that approximately 5% of the U.S. horse population is overweight or obese.[1] The purpose of the present study was to test the hypothesis that there is a greater prevalence of obesity than has been previously reported. Our objectives were to evaluate body condition and determine the prevalence of obesity and hyperinsulinemia in a subpopulation of mature horses in Virginia, measure oxidative stress/inflammatory biomarkers and antioxidant status in this subpopulation, and determine the correlations between these parameters. The subpopulation consisted of 300 mature horses randomly selected the practice area of the Virginia-Maryland Regional College of Veterinary Medicine (VMRCVM). This study was conducted on-farm and body condition scores (BCS) were allotted to each horse, morphometric measurements were taken to determine body weight (BW_{kg}), body mass index (BMI), and blood was sampled to assay for hormones/adipokines (insulin, leptin, and adiponectin), glucose, and oxidative and inflammatory biomarkers (MDA, F_2-Isoprostanes, and TNF-α). It was found that there was a higher prevalence of obesity than previously documented; 47% of the first 100 horses were over weight or obese, 27% were overweight (BCS 6.5-7) and 20% were obese (BCS 7.5-9). Glucose and insulin concentrations increased with increasing BCS. Insulin concentrations were above the normal reference range (8-30 μIU/mL) only in horses with BCS ≥ 6.5, and blood glucose concentrations were within the normal reference range (66-107 mg/dl) for the majority of the horses. BW_{kg}, BMI, and average neck circumference increased with increasing BCS. The current study is relevant to the Virginia horse industry because of the serious health and welfare concerns associated with obesity and its co-morbidities such as laminitis.

NAHMS-USDA (1998). National Animal Health Monitoring System, Equine Mortality and Morbidity Info Sheet. Available at:www.aphis.usda.gov.

Electrospinning of Associating Small Molecules

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ABSTRACT

Electrospinning uses a strong voltage to draw sub-micron diameter sized fibers from a polymer melt. Electrospinning non-covalently associating small molecules, instead of polymers, was investigated. Through such interactions as hydrogen bonding and van der Waal's forces, a sufficient number of entanglements is reached that allows phospholipids and bis-urea organogelators to electrospin successfully. Out of a 4 weight percent solution in 2-butanol, (-)-(S,S)-hexadecyl-3-[2-(3-hexadecyl-ureido)cyclohexyl]urea was successfully electrospun into fibers with unique morphologies, viewed by scanning electron microscopy (SEM). Adding 6 mol water to a solution of phospholipids inhibits electrospinability whereas 3 mol water aides in electrospinning. Rheology data shows that the presence of 3 and 6 mol water creates a shear thickening and shear thinning phenomenon, indicated by a sharp increase then decrease in the viscosity of the system. Rheology data could also help elucidate inhibitory effects water has on phospholipid electrospinability.

Smart Skin for Morphing Wings

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ABSTRACT

The advancement in smart materials has revealed the potential for creating a morphing wing. The dilemma now is finding a material that possesses all the properties needed.

To construct a plane with a morphing wing, a lightweight material with the ability to change area by at least 100% and recover completely after deformation is necessary. The material will need to stand up to aerodynamic forces to avoid dimpling and be able to change from one shape to another quickly with a small force. Using a bi-axial test, a uni-axial tensile test, and a pressure test the mechanical properties were evaluated for a fiber reinforced elastomer material. The fiber used was Nitinol SMA wire, and the elastomer was 3m VHB tape.

Reinforcement of wires showed potential, but more tests with different distributions and configurations is needed. Also testing with different elastomers and fibers is recommended.

R-Ratio Effects on Damage in Fiber Reinforced Polymer (FRP) Composites

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ABSTRACT

Dynamic loading and fatigue failure are some of the largest hurdles to understanding how a material functions. While this has been overcome for metals there is little understanding of how these issues affect fiber reinforced polymer composites. There have been many attempts to predict fatigue lifetimes of fiber reinforced polymer composites. Most of the time statistical analysis is used to try to come up with a quantitative model. This method, coupled with the lack of understanding of damage mechanisms, causes these models to be phenomenological. While this has allowed for use of composites to become more widely available, it fails to increase our understanding of what damage mechanisms are actually occurring. The Materials Response Group has fielded studies that indicate that at different stress levels the damage mechanism that causes failure changes. Knowing what damage mechanisms are causing failure may allow for a more complete model to be formed. Using microscopy these damage mechanisms were examined, looking at R=-1 and R=10. Optical microscopy produced unexpected results that were further looked into using the more powerful SEM. The results clearly show that loading conditions affect the damage mechanisms. The results also lay a foundation for further work and suggest several areas that might produce interesting results when looked into further.

Frequency Effects on Fatigue Life for Vinyl-Ester/E-Glass Structural Composites

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ABSTRACT: Fiber-reinforced polymer (FRP) composites are becoming increasingly popular for use in a variety of civil and naval applications because of the benefits they offer compared to traditional building materials. However, they lack the history of use and research base needed to take them into mainstream use. Research is being done to characterize these FRPs, but much of it occurs at higher frequencies than those experienced in real life applications. This paper focuses on how frequency affects the fatigue life of two Vinyl Ester/E-glass composites, one with 510A as the matrix and the other with elastomer-modified 8084. Tensile tests were performed in order to determine the ultimate tensile strength of each material. A series of constant amplitude tension-tension fatigue tests at various frequencies (0.1, 1, and 10 Hz) and stress levels (21.5, 28, 36.5 ksi) were then carried out to determine the effect of frequency on the fatigue life. The fatigue life is found to increase with increasing frequency in the 0.1 to 10 Hz range for these composites. Temperature increases due to hysteretic heating is not found to have any effect on fatigue life. The 510A matrix composite is found to be stronger and have a longer fatigue life than the 8084 matrix composite.

Structural Fuel Cell Design Using Non-Metallic Substances

By Paul Rodgers, Cory Hilton, Dr. John Lesko, Dr. Scott Case

Abstract

There have been attempts in the past to build proton exchange membrane (PEM) fuel cells that were also capable of carrying mechanical loads. In the past these "structural" fuel cells had been built of metallic materials and were susceptible to corrosion in the fuel cell's aqueous environment. The purpose of this research was to examine ways to replace the metallic materials with more inert non-metallic composites that have the ability to carrying loads while still being able to harness the power generated by the PEM fuel cell. The current results are encouraging when compared to the performance of previous work with metallic "structural" fuel cells. A higher voltage and current density output over previous metallic design have been consistently demonstrated. However, improvements in terms of design can improve upon the data we have already obtained.

Effect of environmental conditions on performance of adhesive joints for infrastructure applications

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Abstract:

This paper presents results from studies on adhesive bonded joints on static and fatigue behavior under different environmental conditions. Adhesively bonded joints composed of FRP composite laminates are currently used on the composite construction. However, there is lack of research on the performance of such joints under environmental conditions such as temperature and moisture. In the current study, most common adhesives for infrastructure application (Pliogrip Polyurethane 7770, Pliogrip Epoxy 5760B from Ashland Chemicals and Magnabond Epoxy A/B from Magnolia Plastic) are chosen for investigation of joint. Joints were tested on a four point bending test until failure (opening of first crack) at quasi-static and fatigue loading conditions. From the results obtained moisture and temperature both have a direct effect on joints showing degradation in stiffness and failure load. However temperature has more effect than moisture showing an average stiffness reduction of 48% and failure load reduction of 67% compare with a stiffness reduction of 20% and failure load reduction of 21% due to moisture absorption. However stiffness degradation is believed to be mostly caused by the loss of stiffness of composite laminate itself and the reduction of failure load is due to degradation of the adhesive system. Fatigue tests are currently in progress.

Creep-Induced Leakage in Proton Exchange Membranes

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Uniaxial creep alone has been shown to induce leakage in proton exchange membranes suspended in high temperature air. This leaking may be relevant to pinhole formation that occurs in operating fuel cells, leading to gas crossover. In order for leaking to occur at 80°C and 5% RH, strains must approach 175%. A portable fixture was developed to conduct in-situ leak rate tests across the membrane. Also, the relationship between applied stress and time to the onset of leaking due to creep has been established.

Dynamic Mechanical Analysis (DMA) of a Moisture Cure Polyurethane Adhesive

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ABSTRACT

Laminated Veneer Lumber (LVL) is an engineered wood composite with several applications in building construction and furniture industry. Currently, LVL is being constructed with a phenol formaldehyde adhesive. This adhesive consumes large amounts of energy to dry the wood and to hot press the composites. In addition to large consumption of energy, the current process releases volatile organic compounds (VOC) from the wood and adhesive. This led to development of a new moisture-cure adhesive. The new adhesive reduces the amount of energy used and the amount of VOC emissions in the production of LVL. This summer small wood bonded samples were constructed with the new adhesive. These samples were tested in a DMA to produce master curves and shift factors. The master curves and shift factors provide information on how the adhesive responds to temperature and how the wood effects the relaxations of the adhesive.

Synthesis of Biocompatible Stabilizers to Tailor the Surface Properties of Magnetic Nanoparticles

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Abstract

The synthesis and characterization of polyether polyurethane homopolymers containing a central block with pendant carboxylic acid groups are discussed herein. Poly(ethylene oxide) (PEO) and poly(propylene oxide) (PPO) homopolymers were synthesized from a benzyl alcohol anionic initiator with varying weight percentages of PEO and PPO. By using benzyl alcohol as the initiator the homopolymers formed had one hydroxyl group at one chain end and a protected hydroxyl group at the other chain end. The polyether polymers were then incorporated into a short polyurethane segment having approximately three carboxylic acid groups per mole. The resulting polyurethane was then subjected to hydrogenolysis to remove the benzyl group and yield primary hydroxyl functionality at the chain ends. Molecular weights determined via ^{1}H NMR were in agreement and close to targeted values demonstrating control over molecular weight. Titrations of the polyurethanes agreed with the targeted value of approximately three carboxylic acid groups per chain.

Threading a Molecular Needle: Complexation Studies of Pseudorotaxanes

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Abstract

Two different host/guest systems are examined in this study. DB30C10 diester (1) with paraquat diol (2) and a functionalized cryptand (3) with dimetyl paraquat (4) were examined by ^{1}H NMR to find the association constant (K_a) of each system. Through graphical methods, the K_{ave} of 1:2 was found to be 38 (± 3) M^{-1} using a Δ_0 of 0.17 ppm. The K_{ave} of 3:4 was found to be 2.3 $(\pm 0.2)\cdot 10^4$ M^{-1} in acetone-d_6 using a Δ_0 of 0.71 ppm. The cryptand was farther studied through the use of X-ray crystallography to demonstrate that the complex was a pseudorotaxane.