THEORETICAL STUDY OF THE EFFECT OF CHAIN SUBSTITUENT MASS ON ENERGY TRANSFER IN COLLISIONS OF Ar WITH MODEL HDPE, PVDF, and PTFE

William A. Alexander and Diego Troya*

Department of Chemistry
Virginia Tech, 107 Davidson Hall
Blacksburg, VA 24061-0212

Abstract

We present a classical trajectory study of energy transfer in collisions of Ar atoms with alkanethiolate self-assembled monolayers (SAMs) with various chain substituent masses. To solely probe mass effects, we alter particle masses within the SAM chains, while holding the interaction potential between the polymers and the noble gas constant. We have utilized these SAMs to construct simple models of three highly crystalline polymers: high-density polyethylene, polyvinylidene fluoride, and polytetrafluoroethylene to investigate at an atomic level the microscopic mechanisms responsible for the superior toughness, chemical and environmental resistance, and durability of fluorinated polymers. Our calculations indicate that an increase in substituent mass results in a decrease of overall energy transfer to the SAM. This is especially apparent when varying substituent mass at the SAM terminus. This trend is qualitatively in agreement with molecular beam experiments, and is a result solely of mass effects. The superior characteristics of fluorinated polymers over those of their hydrogenated counterparts can be attributed to a large degree to projectile/surface mass ratios.

*E-mail: troya@vt.edu

Evaluating DOCK 5.2 for the Analysis of Monoamine Oxidase B and β-Glucosidases

William J. Allen and David R. Bevan
Virginia Polytechnic Institute and State University
Blacksburg, Virginia 24061

ABSTRACT: Computational analysis of ligand-protein interactions, or molecular docking, is an important step towards drug, vaccine, and diagnostic design. One approach is flexible-ligand docking in a grid-based scoring system, as provided by DOCK 5.2. A test set of seven monoamine oxidase B (MAO-B) inhibitors was comprised for molecular docking. Five known ligands and two decoy ligands showed in multiple tests that DOCK can pick out the decoys based on receptor file preparation, including the presence of water in the active site, and docking parameters, including conformational searches, bumps allowed, and unconfined orientation searches. A test set of five β-glucosidase (β-Glu) ligands, some known substrates, and some known to inhibit β-Glu, was also prepared. The study showed that DOCK is able to successfully predict the binding of all test ligands, even with variables like the presence of water in the active site, and in some cases, certain modified residues.

Combined Mechanism Durability Modeling and Validation for Composite Naval Structures

Roberto Alvarado, Richard Speckart, John J. Lesko, Scott Case
Engineering Science and Mechanics Dept.
Virginia Polytechnic Institute and State University
Blacksburg, VA

ABSTRACT

Composite designs have been very rigorous in Naval and Civil applications due to uncertainties of their long-term properties. A design guideline to estimate the changes in the material resistance with time and environmental effects is being developed at Virginia Tech using the Load and Resistance Design Factor (LRFD) approach. This paper focuses on the characterization of the fatigue variability on the Composite Advanced Sail project (CASP) material and compares it to Navy results. A comparison is also made with previous analysis performed on E-Glass/Derakane 510-A laminates. Data showed that the CASP maintained consistent results and its performance differs only slightly with the E-Glass/Derakane 510-A laminates. In addition, the manufacturing process of E-Glass/Derakane 8084 laminates using the Vacuum Assisted Resin Transfer Molding (VARTM) process is described. The results obtained in this study are determinant for further research and important for simulation procedures.

STIMULI RESPONSIVE AMPHIPHILIC TRIBLOCK COPOLYMER BRUSHES

Emily B. Anderson, Kalpana Viswanathan, and Timothy E. Long
Department of Chemistry
Virginia Tech
Blacksburg, VA 24060

Abstract

Stable free radical polymerization enabled the synthesis of polystyrene (PS), polyacetoxystyrene, and poly(*tert*-butyl acrylate) (PtBA) blocks of an amphiphilic triblock copolymer. Poly(styrene-*b*-4-acetoxystyrene-*b*-*t*-butyl acrylate) can surface graft to silicon wafers after central-block silylation. Hydrazine hydrate transformed the acetoxystyrene block to hydroxystyrene; ^{1}H NMR spectroscopy facilitated quantification. Modification of the central hydroxystyrene units with 3-isocyanatopropyl triethoxysilane (IPTES) introduced surface-reactive functionality. ^{1}H NMR spectroscopy and *in situ* FT-IR spectroscopy verified silylation. Functionalized polymer from the melt anchored to silicon surfaces by the central block. The grafting-to approach resulted in Y-shaped copolymer brushes. PS and PtBA formed protruding arms. XPS and water contact angle measurements confirmed the successful modification of silicon surfaces with the triblock copolymer. PtBA block hydrolysis generated poly(acrylic acid) (PAA) under mildly acidic conditions. XPS validated that little or no polymer detached during surface hydrolysis. The PS and PAA rearrangement proved rapid and reversible in solvents of different thermodynamic quality.

Developing a Technique to Characterize Residual Stress in Proton Exchange Membranes

Daniel E. Armanios and David A. Dillard
Department of Engineering Science and Mechanics
Virginia Polytechnic Institute
General Motors Corporation

Abstract

Fuel cells have been shown to be a new and more efficient method to generate power. However, residual stresses in the proton exchange membrane of fuel cells are believed to play a significant role in compromising fuel cell durability. This work employs two conventional and non-destructive methods to characterize the residual stress state of proton exchange membranes, curvature of biomaterial coupons and load-deflection behavior of suspended membranes. Due to poor substrate bonding and complex or poor surface profiles persistent in the biomaterial curvature method, the loading of suspended membranes was explored as another option. The membrane loading method showed more consistent results, but sample preparation was inconsistent due to uncontrollable parameters such as the manufacturing quality of the membranes and the ambient conditions in the room. The lower slope of LiCl treated samples versus the higher slope of the as prepared samples shows that stress relaxation is occurring. A more consistent method of sample fabrication must be found to ensure the success of the membrane method. Once this is optimized, the consistency and test speed of the membrane loading method will serve a successful tool to characterize residual stresses in proton exchange membranes. More selective substrates will have to be used to make the curvature method successful.

Toward Functional Magnetic Nanoparticles for Biotechnology

M.E. Ashworth, M.L. Vadala, Y. Lin, and J.S. Riffle

NSF Summer Undergraduate Research Program
Macromolecules and Interface Institute
Virginia Tech, Blacksburg, Virginia 24061

ABSTRACT

Hydrophilic magnetite nanoparticles are of current interest for biotechnological applications. These macromolecular-magnetite complexes are beneficial due to their ability to disperse in aqueous fluids. An end functional poly(ethylene oxide) (PEO) was designed to synthesize these hydrophilic macromolecular-magnetite complexes. A trivinylsilane and a divinylmethylsilane were synthesized as terminating agents that were directly added to the hydroxy terminus of PEO. ^{1}H NMR confirmed that 60% of PEO chains were functionalized with the trivinylsilane. Carboxylic acid functionality was added to these vinyl end groups via an ene-thiol addition of mercaptoacetic across the vinyl moieties.

Synthesis and Examination of Tri-headed and Two-tailed, Carbamate-linked Ampiphiles

Erika Bechtold, Richard Macri, Woojin Lee, Alan R. Esker, Richard Gandour

Department of Chemistry 0212, Virginia Tech, Blacksburg, Va. 24061

Abstract

A series of tri-headed and two-tailed, carbamate-linked amphiphiles with anti-microbial properties were synthesized with varying hydrophobic chain length to observe the microbial activity as a function of increasing hydrophobicity. A two-step synthesis, with purification of the intermediates, provided high purities and yields for the targetcompounds. Because of their surfactant-like behavior at the air-water interface, Langmuir film studies of the interfacial properties of these amphiphiles was also investigated using the Wilhelmy plate technique and a pH ≈1 acid subphase. All of the amphiphiles formed liquid-expanded (LE) monolayers; lift-off, extrapolated limiting areas and collapse concentrations gave values on the order of $A_{liftoff}$ = 115, A_0 = 95 , and $A_{collapse}$ = 60 $Å^2$/molecule respectively.

CONTROLLED DEPOSITION OF CELLULOSE NANOCRYSTALS USING INK-JET PRINTING TECHNOLOGY

Jessica Bradford and Maren Roman
Department of Wood Science and Forest Products
Virginia Tech
Blacksburg, VA 24061

Abstract

Suspensions of cellulose nanocrystals form colloidal chiral nematic phases that can be captured in iridescent thin films. These films have a number of potential applications in counterfeiting prevention, decorative coatings, biomedicine, and micro-optics. Ink-jet printing has attracted attention as a potential method for depositing these films due to its precision, affordability, and reproducibility. Here, we tested ink-jet printing for the deposition of cellulose nanocrystals onto glass substrates. We also investigated the effect of different cleaning methods for the glass substrates. We used atomic force microscopy to characterize individual nanocrystals and deposit topography. We used polarized-light microscopy to observe the drying patterns produced by droplets of nanocrystal suspension. We determined that ink-jet printing could successfully deposit cellulose nanocrystals in a controlled and reproducible pattern; however, we did not observe any self-assembled structures.

CHARACTERIZATION OF PROTON EXCHANGE MEMBRANES FOR FUEL CELLS

Alicia Castagna*, Linda Harris, Abhishek Roy, James McGrath
Macromolecules and Interfaces Institute
NSF Summer SURP Program*
Virginia Polytechnic Institute and State University
Blacksburg, Virginia

Abstract

Poly(arylene ether sulfone)s (BPS) are ideal materials for proton exchange membranes (PEMs). Moderate molecular weight (25K) acidified BPSH films with 35 mol% disulfonation were investigated. The effect of membrane thickness on fuel cell performance was studied, and it was found that with increasing thickness the cell resistance increases. In addition, the performance improves with decreasing thickness to an extent. Cell resistance data was used to determine the true proton conductivity of the membrane in the membrane electrode assembly (MEA). The effect of varying the processing temperature of the MEAs influence on performance was also investigated. The effects of the processing temperature and film thickness were quantified using fuel cell performance curves and high frequency resistance values.

Mechanical property evaluation of fire retardant resins

Brian Clements, John Bausano, John J. Lesko, Scott Case
National Science Foundation (NSF)
Department of Engineering Science and Mechanics
Materials Response Group
Virginia Polytechnic Institute and State University
Blacksburg, Va 24061

Abstract

The use of fire retardant resins is important to the advancement of composite technology. It is necessary to create fire retardant composites that do not exhibit significant loss in mechanical properties when compared to their non-fire retardant counterparts. This would allow the use of composites in a wider range of applications. The purpose of this paper is to compare the properties of a control S 2 glass/SC15 composite against a brominated S 2 glass/SC15 composite. The completion of tension and compression tests allowed us to compare material properties such as modulus of elasticity, ultimate compressive strength, and ultimate tensile strength. The control composite also underwent mode I and mode II fracture toughness tests. Experimental results showed that there was no significant loss in the mechanical properties of the fire retardant composite and in some instances, there was even an increase in the mechanical properties of the fire retardant composite. Further testing will allow us to compare the fracture properties of the two composites.

DURABILITY AND PERFORMANCE OF EPOXY BONDED TO ALUMINA UPON IMMERSION IN AQUEOUS SOLUTIONS

Jacquelyn Evans and John Dillard
Macromolecules and Interfaces Institute
Department of Chemistry
Virginia Polytechnic Institute and State University
Blacksburg, VA 24061

Abstract

The durability of an epoxy-aluminum bonded system was evaluated upon immersion in aqueous solutions. The surface modification of an aluminum bar to replicate the surface of an alumina bar is discussed. The modifications performed were an iron(III) sulfate (Fe(III)/Al) treatment and an aluminum oxide-grit blasting followed by an iron(III) sulfate (Al_2O_3 GB/Fe(III)/Al) treatment. A bonded joint system created by adhering two modified aluminum bars with an amine cured epoxy was subjected to wedge testing. Wedge specimens were immersed in aqueous solutions at pH 4 and pH 9, at room temperature and at 70 ˚C. The Fe(III)/Al specimen showed the best performance at room temperature with low crack growth and cohesive failure in the adhesive. The Al_2O_3 GB/Fe(III)/Al sample showed improved performance at 70 ˚C relative to the Fe(III)/Al specimen with a lower amount of crack growth and resistance to adhesive failure. The pH 4 solution was the more aggressive of the two solutions in that it caused adhesive degradation as indicated by browning and flaking of the epoxy. The tests at elevated temperature resulted in increased bond degradation in both solutions.

Genetic Regulation of Embryo Development in *Pinus taeda*

Jackeline Hamelius and Supriya Ratnaparkhe
Dr. Ulrika Egertsdotter
Department of Forestry
Virginia Tech 24060
Blacksburg, Virginia

Abstract

The genes that this study undertook; BLADE ON PETIOLE1 (BOP1), SHEPHERD (SHD), and the five Matrix metalloproteinases (MMPs), play a significant role in growth and development of embryos and physiological processes. The process of somatic embryogenesis (SE) is a technique that holds the potential to mass-produce genetically identical engineered trees like loblolly pine (*Pinus taeda*). As a result, this technology will increase the productivity and sustainability of the forestry industry. Genes BOP1 and SHD, represent suppressor genes that promote leaf development. Although the five MMPs expression occur at a later stage of development, they still play an important role in growth factors and morphogenesis. In our research, we searched the *Arabidopsis thaliana* sequence database for these particular genes and searched for homology alongside loblolly pine expressed sequence tag (EST) DNA library. The conserved regions of the MMPs such as the cysteine residue and the zinc-binding motif were used to find homology with loblolly pine.

Oxidative damage and antioxidant status in the canine diabetic and non-diabetic cataractous lens

Anya C. Hawthorn, MS
Faculty Mentor: Dr. Korinn Saker, DVM, PhD, DACVN

Abstract

This study quantifies levels of the antioxidant enzymes glutathione (GSH), glutathione peroxidase (GPX), superoxide dismutase (SOD) and catalase within the healthy canine lens and within the canine diabetic and nondiabetic cataractic lens. Antioxidant enzyme levels were also measured within peripheral white blood cells (WBCs) as a measure of systemic antioxidant status. Lenses were assayed for oxidative damage to proteins in the form of increased protein carbonyl content and for lipid peroxidation by quantification of malondialdehyde (MDA). SOD was not detectable in healthy or cataractic canine lenses, although a trend towards decreased levels of SOD in peripheral leukocytes of dogs with cataracts was observed. Dogs with cataracts displayed decreased peripheral leukocyte levels of GPX and GSH; however, cataractic lenses had significantly increased levels of both these enzymes as compared with healthy lenses. Canine cataracts have elevated levels MDA, indicating lipid peroxidation, but protein carbonyl content was not significantly different between healthy and cataractic lenses.

Dogs may be uniquely able to induce GSH and GPX in lens tissue during the process of oxidative stress that leads to cataract development, although it seems likely that most of the glutathione present in the cataractic lens is in the oxidized form.

Deglycosylation of Flavonoids by Lactic Acid Fermentation in Air and Reduced Oxygen Atmospheres

Ayaka Honda. Dr. Susan Duncan. Kim Waterman.
Department of Food Science and Technology
Virginia Polytechnic Institute and State University
Blacksburg, Virginia 24061

Abstract

This study was undertaken to investigate the application of ß-glucosidase-producing lactic acid bacteria as an enzyme pathway to deglycosylate the soy isoflavonoids in Easy Soy® supplement through a yogurt fermentation system. The hydrolysis reaction converts the glycone form genistin, an isoflavonoid commonly found in soy, to its aglycone form genistein. Genistein is believed to be the more bioavailable form of the two isoflavones. The effect on yogurt quality, yogurt culture bacterial survival, oxidation, and rate of deglycosylation is measured by setting up four different yogurt treatments. The four treatments were control with air flush, control with nitrogen flush, flavonoid- fortified with air flush, and flavonoid- fortified with nitrogen flush. The nitrogen flush treatments were sealed in oxygen barrier ethylene vinyl alcohol polypropylene cups and the air flush in regular polypropylene cups. Sensory and textural effects from the treatments were minimal. 5 sensory panelists noticed a slight hay like flavor from the flavonoid, but it was not strong enough to discourage consumption of the product. Overall, slight textural changes were noticed. For bacterial survival of the yogurt culture, the flavonoid fortified treatments inhibited survival of total lactics and *L. acidophilus* by almost a log order, but promoted survival of *B. lactum* by almost a log order. Glucose and HPLC results were inconclusive, but with continued research, hope to satisfy the hypothesis. The flavonoid and nitrogen conditions reduced oxidation in yogurt with implications for greater use of antioxidants in the dairy industry for prolonged shelf life.

pH and Ion Effects on Trisilanolphenyl-POSS Stability

Sarah M. Huffer, Kevin J. Dawson, Jianjun Deng, Suolong Ni, and Alan R. Esker
Department of Chemistry, Virginia Polytechnic Institute and State University
Blacksburg, Virginia 24061

Abstract

Polyhedral oligomeric silsesquioxanes (POSS) have been an innovative area of intense study for the past two decades. In this study, trisilanolphenyl-POSS (TPP), a molecule known to form Langmuir films at the air/water interface, was examined for stability at various pH values. Isothermal and isobaric experiments using the Wilhemy plate technique along with Brewster angle microscopy (BAM) images were used to investigate the stability of TPP on buffered subphases. This study found that the stability of TPP decreased as the basicity of the subphase increased. As the TPP rested on the subphase, hydrolysis reactions cleaved siloxane bonds and dissolution into the subphase occurred. Bicarbonate anions in the buffered subphases at pH = 10 and pH = 11 decreased the stability of TPP and affected the rates of hydrolysis and desorption relative to borate and phosphate buffers, respectively.

UV-Curable Cationic Polyelectrolytes for Electrospun Antimicrobial Membranes

Peter Jian, John M. Layman, and Timothy E. Long
Virginia Polytechnic Institute and State University
Blacksburg, Virginia 24061

Abstract:

A novel polymeric fiber was fabricated from poly(dimethylaminoethyl mathacrate-co-hydroxy mathycrate) (PDMAEMA-co-HEMA), and its cell cytotoxicity activity was assessed. PDMAEMA-co-HEMA was synthesized from DMAEMA and HEMA via free radical polymerization. This polymer was protonated in hydrochloric acid to give a polyelectrolyte. This polyelectrolyte was functionalized with cinnamoyl chloride, a UV-curable photocrosslinker. Next, the functionalized polyelectrolyte was electrospun to form sub-micron-sized fibers. Finally, cell cytotoxicity demonstrated the antimicrobial activity of this fiber using mouse neuroblastoma cells.

FLEXURAL RESPONSE OF UNDER AND OVER REINFORCED GLASS FIBER-REINFORCED POLYMER (GFRP) REINFORCED CONCRETE BEAMS

Ileaner V. Maldonado- Antonio, Theophanis Theophanous
Dr. Carin Roberts-Wollmann, Dr. John J. Lesko and Dr. Scott Case.
National Science Foundation (NSF)
Department of Engineering Science and Mechanics
Virginia Polytechnic Institute and State University
Blacksburg, VA 24061

Abstract

Steel Corrosion repair is becoming more costly everyday; as a result of this, composites are being used more widely for construction. One example of this is Glass Fiber Reinforced Polymers (GFRP), they offer light weight construction, resistant to corrosion, strength greater than steel, among other benefits. GFRP bars exhibit a very brittle and sudden failure at tension, while steel yields before failure allowing for deformations to occur on a beam before failure. Since GFRP bars do not yield and fail so suddenly, not allowing for deformations to take place, engineers are very conservative when they design GFRP reinforced beams. They design them to be over reinforced in most cases. Our goal through this effort is to asses the reliability of under and over reinforced GFRP beams. 15 GFRP bars were tested in tension from the same lot as the bars used to build the beams. Stress vs. strain curve was plotted and maximum strength and Modulus of elasticity was calculated for bars to get the average and standard deviation. All 4 beam where tested under flexion by simply supporting the beams and applying a single load at the mid span. All beams where loaded until failure, deflection vs. load plots where analyzed and flexural strength was calculated and compared to the ACI 440 standards. GFRP bars exhibit a great variability within a lot. Theoretical model of flexural behavior of GFRP beams does a very good job at predicting the experimental

behavior up to and close to failure, but is not as good when predicting behavior for the beginning of the test. Results from this work will be added to the effort of validating the existing design code for FRP, ACI 440.

STABILITY OF ETHYL-*t*-BUTYL ETHER LEACHED FROM POLYETHYLENE PIPES BY DRINKING WATER

Julie Martin, Monique Durand, Andrea M. Dietrich
Civil and Environmental Engineering
Virginia Tech
Blacksburg, VA 24061-0246

Abstract

Previous research found ethyl-*t*-butyl ether (ETBE) in drinking water after exposure to cross-linked polyethylene (PEX) pipes. Water with chlorine or chloramines disinfectant showed lower concentrations of ETBE than water without disinfectant after three days of exposure to PEX. This study focused on the relationship between the concentrations of ETBE in water with chlorine and no disinfectant to determine (1) whether the presence of chlorine contributed to the degradation of ETBE over three days or (2) if the analytical method used to detect ETBE was affected by the presence of chlorine. Statistical analysis of the data showed no change in the concentration of ETBE over three days for water samples with chlorine or no disinfectant. However, the data trends suggest that the chlorinated samples had a lower concentration of ETBE than those in the absence of disinfectant. Further research is needed to investigate this relationship.

STRUCTURE-MECHANICAL PROPERTY RELATIONS FOR CHARRED COMPOSITE MATERIALS

Michael A. Meneses Lopez, Kai Zuehlke, Dr. John J. Lesko, Dr. Scott Case

National Science Foundation
Department of Engineering Science and Mechanics
Material Response Group
Virginia Polytechnic Institute and State University
Blacksburg, VA 24061

ABSTRACT: The use of composite insulators for rocket motor insulation has grown in the past years. This is greatly due to the fact that composite insulators possess superior insulation behavior and adds almost no weight to the motor, which is the goal in the designing process. The main problem involves premature mechanical erosion in the charred state. Usually the mechanical properties are ignored; this can lead to various problems, including over design. This paper presents the work done with three different charred Kevlar/EPDM rocket motor insulating materials; designated ARI-2718, ARI-2719, and ARI-2750. It consisted in developing an understanding of the properties of the charred insulating materials including microstructure and composition, thermal properties, and mechanical properties. The microstructure study, using SEM/EDS, showed that ARI-2750 contains Aluminum, instead of Silica, which the other materials possessed. Tests performed using the Hot Disk show that the thermal properties of the materials decrease with charring. The ARI-2750 was the only material stable enough to withstand the sample preparation process for mechanical properties testing. We hypothesize that the aluminum, in its oxidized state, possessed by the ARI-2750 makes it stronger than the other materials. Dynamic Mechanical Analysis (DMA) testing which focused on shear strength, done on both fiber orientations (0 and 90 directions) of the ARI-2750, showed that the greatest shear strength lies in the 0-direction, with 190 kPa shear strength. In addition, this paper includes the work done on woven glass/vinyl ester resin material, which is used by the Navy for ship decks. The work consisted of a study of the material's behavior in fire conditions. The study was performed by using the Hot Disk, which showed that the thermal properties of the material decreases with decomposition. The data obtained in this study will serve as input for micro-mechanical modeling that will serve to assess how the charred materials' properties can be improved.

TESTING AND CHARACTERIZATION OF POLYMERIC SENSORS ON BEAMS

Emmanuel Padilla Salinas, Miles Buechler

Supervisors: Dr. Don Leo, Dr. Jack Lesko, and Dr. Scott Case

Integrated Graduate Education and Research Traineeship (IGERT), Research Experience for Undergraduates (REU) Programs of the National Science Foundation (NSF)

Center for Intelligent Materials System and Structures (CIMSS)

Material Response Group (MRG)

Department of Engineering Science and Mechanics

Virginia Polytechnic Institute and State University

Blacksburg, VA 24061

Abstract

The CIMSS lab at Virginia Tech has developed a new class of polymeric sensors that measure the mechanical strain in materials. The goal of this project will be to characterize the sensitivity of these polymeric sensors and compare them with the more conventional piezoelectric films. For this a setup of a cantilever beam is designed and analyzed according to the mechanics of the beam and boundary conditions. This analysis is necessary to validate the electrical response measured by the polymeric sensors. The second phase of the project consists on comparing the polymeric sensor signal directly to the signal output of a piezoelectric film. The end result of this project will be a better understanding of the sensitivity of this new class of

polymeric sensors and a direct comparison of the electrical output with piezoelectric films. Tests show us that this type of sensor does work as a strain gage although the manufacturing technique needs to be improved. The sensor sensitivity on these polymers is a function of the frequency as expected with polymeric materials. Also the output signals of the polymeric sensors tended to be stronger, meaning an increase in sensitivity when compared to piezoelectric films.

FRACTURE RESISTANCE OF PROTON EXCHANGE MEMBRANES

Jennifer Quincy, Yongqiang Li, David Dillard
National Science Foundation
Summer Undergraduate Research Program (SURP)
Department of Engineering Science and Mechanics Virginia Tech
Blacksburg, VA 24061

Abstract

Intrinsic fracture energy, an inherent property of a material, is the energy required to break the chemical bonds of the material per unit of fracture area. This is the lowest energy required to cause failure in the material. Plastic deformation in the material increases measured fracture energy. This fracture energy experiment minimized plastic deformation by applying a sharp blade to the crack tip. A stationary razor blade cut membrane samples at constant angles and rates. The slitter structure held the membrane away from the blade, minimizing frictional effects. Fracture energies measured at two temperatures, four humidity levels, and five cutting rates reveal viscoelastic behavior of the membrane. Time-moisture superposition analysis predicts the behavior of membranes at a range of rates beyond the experimental limitations. Fracture energies were calculated using Lake and Yeoh's[1] fracture energy approach to fracture mechanics. An unpredicted angle dependence was observed when different geometries were tested. Nonetheless, this method exhibits significant promise, producing repeatable results for fracture energies nearly two orders of magnitudes smaller than those obtained using tear tests. Shifting the data produced reasonable master curves that were consistent with expected behavior. It is anticipated that this experimental technique can be extended to a range of testing conditions and PEM materials.

Proposed Concrete Filled Fiber Reinforced Polymer (CFFRP) Tube Aging Study

Kelvin Santiago, Jason Cain, John Lesko and Scott Case
Department of Engineering Science and Mechanics
Materials Response Group
Virginia Tech, Blacksburg, VA

ABSTRACT

Protecting concrete columns against corrosion and improving their resistance at the same time is something to look forward to in every structure. Fiber reinforced polymer (FRP) tubes provide a new promising way to accomplish this task. Using FRP as a confinement product for concrete requires a better understanding of how the properties of the material change over time. Testing the material on tension, compression and hoop tension must be performed over a long period of time to understand its behavior. In order to simulate the effect of age, hygrothermal aging is used. Three different conditions are used and compared to baseline samples. This allows simulating property and durability changes on the material. Developing a model for durability is the final goal of this study. In order to perform testing on FRP sample tubes, methods to fit the form and curvature of the tube are required. A comparison of the unaged and aged sample is performed. A new method currently under development is proposed.

The Synthesis and Characterization of Linear Poly (D,L-lactide)s Containing Pendant Complementary Multiple Hydrogen Bonding Groups

Joycelyn S. Smith, Afia S. Karikari, and Timothy E. Long
MILES/IGERT
Department of Chemistry
Virginia Polytechnic Institute and State University
Blacksburg, VA 24061

Abstract:

A series of poly (d,l-lactide)s (PDLLA) with molar masses ranging from 8,000 to 60,000 g/mol were synthesized with a poly(ethylene glycol) methyl ether and poly(ethylene glycol) to achieve monofunctional and difunctional linear polymers respectively. The hydroxyl endgroups were functionalized with acryloyl chloride to achieve acrylated end groups. The acrylated end groups were further modified with complementary hydrogen bonding groups such as adenine and thymine via Michael addition. ^{1}H NMR, SEC, TGA, solution rheology and melt rheology were used to characterize and probe the effect of hydrogen bonding and molecular recognition in these linear PDLLAs. A solution blended system consisting of 50:50 mixture of the adenine and thymine modified polymers, PDLLA-ADE and PDLLA-THY respectively, demonstrated thermoreversibility. Solution rheology analysis revealed a significant increase in viscosity for the PDLLA-A and PDLLA-T mixture compared to a non-blended system.

Investigation of Dewetting within Thin Polymer Bilayer Films

Michael C. Swift, Rituparna Paul, John R. Hottle and Alan R. Esker

Department of Chemistry
Virginia Tech, Blacksburg, VA 24061
miswift@vt.edu, rpaul@vt.edu, hottle@wisc.edu and aesker@vt.edu

Polymer thin films have found many uses in today's technology. However, problems such as dewetting of the thin films above the polymer's glass transition temperature as well as a co-existence of dewetting and phase separation have been observed. Polymer bilayers have been one of the areas of experimentation to further investigate these properties. In this study, a bilayer film consisting of a polymer, polystyrene (PS), and a model nanofiller, trisilanolphenyl-POSS (TPP), will be used to study how nanofillers influence stability and wetting in thin film systems. The bilayers were prepared using spincoating (PS) and the Langmuir-Blodgett (LB) technique (TPP) to investigate the nature and mechanism of dewetting and its effects on the morphology of the bilayer films at elevated temperatures. Optical microscopy (OM), X-ray photoelectron spectroscopy (XPS), and atomic force microscopy (AFM) were used to investigate the morphology as a function of annealing temperature and time. For annealing at 200 ºC, results show that dewetting starts in the upper TPP layer and eventually also occurs in the lower PS layer. Both layers ultimately dewet revealing the elemental Si substrate underneath. After sufficiently long annealing times (~110 min) at 200 ºC, PS forms isolated droplets on the Si substrate. XPS results show that these PS droplets are encapsulated in TPP. Based on OM and AFM images, stresses arising from the diffusion of PS into the rigid TPP, lead to cracks along hexagonal patterns that ultimately serve as nucleation sites for dewetting.

Ian Winters
SURP Virginia Tech
10/24/2005

"Analysis of the Repeatability of Techniques Used to Measure the Stress Relaxation and Creep Compliance of Nafion Membrane"

Author: Ian Winters,
Virginia Tech, SURP Participant
University of Tennessee, Mat. Sci. and Engr.

ABSTRACT

In the search for a more environmentally friendly alternative to internal combustion engines, much research has focused on fuel cells. The most actively research fuel cell for use in the automotive industry is the Proton Exchange Membrane (PEM) fuel cell, also known as Polymer Electrolyte Fuel Cell (PEFC). Nafion is one PEM under consideration for use in PEFCs. However, before the employment of Nafion for wide commercial use, more knowledge of its mechanical properties is required. For example, the techniques used to analyze those properties require analysis. In situations of instantaneous stress and/or loading, stress relaxation and creep tests are the most commonly used testing methods. Samples of Nafion membrane were tested in a Dynamic Mechanical Analyzer (DMA), three times under stress relaxation (0.5% strain) and three times under creep compliance (stress temperature dependent). The humidity was ambient and the temperature was step increased from 30 ºC to 120 ºC in 5 ºC increments. After analysis of the loss tangents, shift factors, and master curves of the different tests, it has been concluded that stress relaxation is a much more reliable and repeatable data collection method than creep compliance.