

SIXTY-FIRST ANNUAL MAY CONFERENCE

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**The Cleveland Section of the
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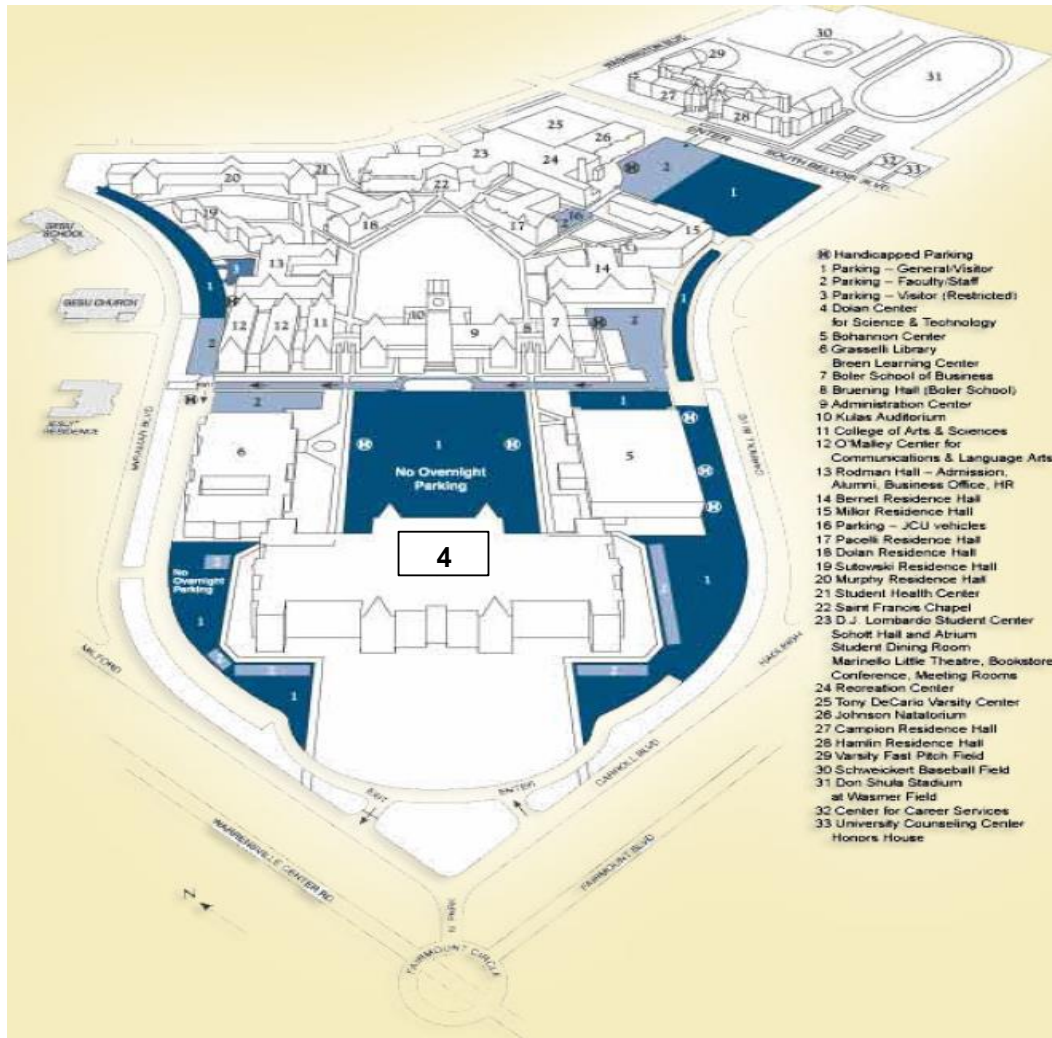
**The American Vacuum Society,
Ohio Chapter**



May 24, 2017

**Dolan Science Center
John Carroll University
University Heights, Ohio**

John Carroll University Campus Map



**61st Annual
SAS / MSNO / ACS / AVS May Conference**

**May 24, 2017
John Carroll University
Dolan Science Center**

PROGRAM

- 7:30 a.m.** **Registration/Continental Breakfast:**
(Edward M. & Ann Muldoon Atrium)
- 8:30 a.m.** **Opening Remarks:** (Donahue Auditorium)
Brian Perry, *LORD Corporation*
Mike Setter, *John Carroll University*
- 8:45 a.m.** **Keynote Address:** (Donahue Auditorium)
Chair: Regan Silvestri, *Lorain County Community College*

George S Bullerjahn – *Bowling Green State University*

“Cyanobacterial blooms in Lake Erie – is there ANY good news?”
- 9:35 a.m.** **Break (15 minutes):** (Edward M. & Ann Muldoon Atrium)

Presentation Session I

	Session IA Dolan A202 Chair: Janet Gbur	Session IB Dolan A203 Chair: Sandra Pejic	Session IC Dolan E130 Chair: Wayne Jennings
9:50 a.m.	IA-1 Dustin Tyler “Sensory, Motor, System: Creating a Replacement Sensorimotor System for Prosthetics” <i>Case Western Reserve University</i>	IB-1 Bjorn Lussem “Minority and Majority Currents in Doped Organic Transistors” <i>Kent State University</i>	IC-1 Denise Inman “Tracking Organelles in the Visual System: Insight into Mechanisms of Glaucoma” <i>NEOMED</i>
10:15 a.m.	IA-2 Michael Presby “Characterizing Impact Damage of Ceramic Matrix Composites using Micro-Computed Tomography and Optical Microscopy” <i>The University of Akron</i>	IB-2 Devesh Dadhich Shreeram “Synthesis and Characterization of Pulse Reverse Current Based Electrodeposited Ni-W Coatings” <i>The University of Akron</i>	IC-2 Kendall Hoover “Role of the Crimpy-Gbb Signaling Pathway at Synapses” <i>Case Western Reserve University</i>
10:40 a.m.	IA-3 Daniel F. Lawrence “Atom Probe Tomography: Technology and Applications” <i>CAMECA Instruments, Inc.</i>	IB-3 Veronica Livingstone “One-Pot in-situ Preparation of Polypyrrole Composites with Metal Oxide Fillers” <i>The University of Toledo</i>	IC-3 Sofia Chinchilla “Quantification and Characterization of Coronary Collateral Arteries using Micro-Computerized Tomography (CT)” <i>NEOMED</i>
11:05 a.m.	IA-4 Harry Scott “Cryo-electron Microscopy Reveals an Anthrax Pore Intermediate” <i>Case Western Reserve University</i>	IB-4 La'Nese Lovings “Synthesis and Characterization of Al _x Sc _{2-x} Mo ₃ O ₁₂ Using Non-Hydrolytic Sol-Gel Methods” <i>The University of Toledo</i>	IC-4 Diane Smith “Capture of Mycobacterium Smegmatis mc(2)155 on Alumina and Silica Substrates of Various Surface Potentials” <i>The University of Akron</i>

11:30 a.m. Break (15 minutes): (Edward M. & Ann Muldoon Atrium)

11:45 a.m. SAS National Distinguished Service Award – Brian Perry
Chair: Regan Silvestri, *Lorain County Community College*

11:55 a.m. Yeager Award: (Donahue Auditorium)
Co-Chairs: Rick Kus, *De Nora Tech, LLC*
Michael Levy, *ACS Chair-Elect – Envantage, Inc.*

Rachel Molé, *The College of Wooster*

“Assessing Load Reduction of Pharmaceutical Compounds in Effluent Post-Disinfection at Chicago’s O’Brien (UV) and Calumet (ClO⁻) Water Reclamation Plants: HPLC-MS/MS Analysis of Effluent Combined with Bench-Scale Simulations”

12:30 p.m. Lunch: (O’Connell Reading Room)

1:00 - 2:00 p.m. Poster Session: (Second Floor Hallway)

Presentation Session II

	Session IIA Dolan A202 Chair: Dingqiang Li	Session IIB Dolan A203 Chair: Regan Silvestri	Session IIC Dolan E130 Chair: Zhorro Nikolov
2:00 p.m.	IIA-1 Dalia Yablon "Advances in Atomic Force Microscopy (AFM) Based Methods to Characterize Polymer Materials on the Nanoscale" <i>SurfaceChar LLC</i>	IIB-1 Brandon Holcomb "Analysis of a Novel Mutation Located in the ccr5 Gene with Potential Effects on HIV Infectivity" <i>Lorain County Community College</i>	IIC-1 Mark Foster "X-ray and Neutron Scattering Studies of Confinement Effects in Polymer Thin Films" <i>The University of Akron</i>
2:25 p.m.	IIA-2 Mohamed ElKabbash "Ultrathin Nanometer Scale Absorber Using Lossless Dielectric and Low Conductivity Metal" <i>Case Western Reserve University</i>	IIB-2 Tin Phan "Characterizing the Effects of the Delta32 Mutation Found from Yersinia Pestis Survivor Descendants on CCR5 Expression and HIV Infectability" <i>Lorain County Community College</i>	IIC-2 Jonathan Cowen "Crystallite Size Analysis of Nanomaterials by X-ray Diffraction" <i>Case Western Reserve University</i>
2:50 p.m.	IIA-3 Alex Nyarko "Understanding the Chemical Composition of the Caulobacter Crescentus Adhesive Holdfast" <i>The University of Akron</i>	IIB-3 Chad Coolidge "Carbon Nanotubes Improving Activated Carbon as a Filter Media" <i>Lorain County Community College</i>	IIC-3 Javier Esquivel "Study of Solid Solubility and Grain Size of Mechanically Alloyed Al alloys Utilizing X-Ray Diffraction Analysis" <i>The University of Akron</i>
3:15 p.m.	IIA-4 Kyle Whiddon "Quantification, Characterization, and Simulation of the Intracytoplasmic Membranes of Methanotrophic Bacteria by Fluorescence Microscopy" <i>The University of Akron</i>	IIB-4 Valerie Gardner "GC-MS Analysis of Unprecedented Whiskey Flavors Including Chinese Baijiu Flavored as American Bourbon" <i>Lorain County Community College</i>	IIC-4 Jeffrey Nantais "Residual Stress Measurements in Automotive Components via X-Ray Diffraction" <i>Proto Manufacturing</i>

3:40 p.m. Break (20 minutes): (Edward M. & Ann Muldoon Atrium)

Presentation Session III

	Session IIIA Dolan A202 Chair: Ron Raleigh	Session IIIB Dolan A203 Chair: Robert Williams	Session IIIC Dolan E130 Chair: Rick Kus
4:00 p.m.	IIIA-1 Ben Xu "The Fundamentals of Rheology and the Application in PSA" <i>Avery Dennison Corporation</i>	IIIB-1 Selim Gerislioglu "Site-Specific Characterization of PEGylated Insulin Isomers by Using Combined Liquid Chromatography and Ion Mobility Mass Spectrometry" <i>The University of Akron</i>	IIIC-1 Jennifer Peverelle "Microstructural Analysis of Welding Slags" <i>The Lincoln Electric Co.</i>
4:25 p.m.	IIIA-2 Saranshu Singla "Adhesion under Humid Conditions: Lessons from Spider Silk" <i>The University of Akron</i>	IIIB-2 Savannah Snyder "MALDI-MS/MS to Determine Sequencing Information of Novel Side Chain Liquid Crystalline Copolymers" <i>The University of Akron</i>	IIIC-2 Louis Ray "Detection of Membrane and Cell Wall Targeted Antibiotics Using RedoxSensor Green™" <i>The University of Akron</i>
4:50 p.m.	IIIA-3 Michael See "Liquid Additives for Plastics Injection Molding" <i>Member of Cleveland Chapter SPE</i>	IIIB-3 Matt Bartucci "Using Infrared and Raman Microscopy to Correlate Visual Images to Chemical Composition" <i>Thermo Fisher Scientific</i>	IIIC-3 Warren MoberlyChan "Low Voltage EDS using Windowless EXTREME Detector" <i>Oxford Instruments</i>

5:15 - 7:00 p.m. Reception/Program

Chair: Brian Perry, *LORD Corporation*

Recognition of Meeting Sponsors

Rick Kus: *DeNora Tech, LLC*

Bell Award Presentations

Tom Steele: *SAS Member, Chemistry Professional*

Best Student Poster Awards

Tom Steele: *SAS Member, Chemistry Professional*

Best Student Paper Awards

Regan Silvestri: *Lorain County Community College*

MSNO Student Awards

Min Gao: *Kent State University*

Raffle

Janet Gbur: *Case Western Reserve University*

Closing Comments

Brian Perry: *LORD Corporation*

2017 May Conference Planning Committee

General Committee	Brian Perry, LORD Corporation Amir Avishai, Case Western Reserve University Coleen McFarland, Envantage, Inc. Min Gao, Kent State University Rick Kus, De Nora Tech, LLC Regan Silvestri, Lorain County Community College Doug Rhode, Lake County Crime Laboratory Mike Setter, John Carroll University Tom Steele, SAS Member Hao Qu, Momentive Performance Materials Bob Williams, SAS Member Nanthawan Avishai, Case Western Reserve University Zhorro Nikolov, The University of Akron Ina Martin, Case Western Reserve University Janet Gbur, Case Western Reserve University
Corporate Sponsors	Rick Kus, De Nora Tech, LLC Nanthawan Avishai, Case Western Reserve University Bob Williams, SAS member Hao Qu, Momentive Performance Materials
Technical Program	Min Gao, Kent State University Brian Perry, LORD Corporation Regan Silvestri, Lorain County Community College Nanthawan Avishai, Case Western Reserve University Zhorro Nikolov, The University of Akron Rick Kus, De Nora Tech, LLC Janet Gbur, Case Western Reserve University
Publicity	Min Gao, Kent State University Brian Perry, LORD Corporation Janet Gbur, Case Western Reserve University Coleen McFarland, Envantage, Inc.
Finance	Bob Williams, SAS Member Hao Qu, Momentive Performance Materials
Registration	Nanthawan Avishai, Case Western Reserve University Hao Qu, Momentive Performance Materials Amy Carlton, De Nora Tech, LLC Rick Kus, De Nora Tech, LLC Danqi Wang, Case Western Reserve University
E. B. Yeager Award	Rick Kus, De Nora Tech, LLC Mike Dowell, Akron ACS Doug Rohde, Lake County Crime Laboratory
Student Paper Awards	Reagan Silvestri, Lorain County Community College Melanie Knowlton, LORD Corporation Ina Martin, Case Western Reserve University Robert Williams, SAS member

	Zhorro Nikolov, The University of Akron Wayne Jennings, NASA-Glenn Ron Raleigh, Byk Additives and Instruments Dingquiang Li, Youngstown State University Sudheer Molugu, Case Western Reserve University Xiaoting Gu, Case Western Reserve University
Student Posters	Tom Steele, SAS, Chemistry Professional Kevin Otteni, LORD Corporation Matt Moesta, LORD Corporation Coleen McFarland, Envantage, Inc. Lu Zou, Kent State University
MSNO Student Awards	Min Gao, Kent State University Nanthawan Avishai, Case Western Reserve University Lu Zou, Kent State University Danqi Wang, Case Western Reserve University Ina Martin, Case Western Reserve University Zhorro Nikolov, The University of Akron Dingquiang Li, Youngstown State University
John Bell Award	Tom Steele, SAS Member Brian Perry, LORD Corporation Rick Kus, De Nora Tech, LLC
Poehlman Award	Coleen McFarland, Envantage, Inc.
Abstract Booklet	Brian Perry, LORD Corporation Rick Kus, De Nora Tech, LLC Melanie Knowlton, LORD Corporation

Society for Applied Spectroscopy

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VICE-PRESIDENT	Thomas Steele, SAS, Chemistry Professional
SECRETARY	Coleen McFarland, Envantage
TREASURER	Robert Williams, SAS Member

Microscopy Society of Northeast Ohio

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TRUSTEE	Min Gao, Kent State University
TRUSTEE	Zhorro Nikolov, The University of Akron
TRUSTEE	Ina Martin, Case Western Reserve University
STUDENT COMMITTEE MEMBER	Janet Gbur, Case Western Reserve University
STUDENT COMMITTEE MEMBER	Gaurav Amarpuri, The University of Akron

American Chemical Society

CHAIR	Lisa Ponton, Baldwin Wallace University
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SECRETARY	Drew Meyer, Case Western Reserve University
TREASURER	John Moran, Notre Dame College

AVS, Ohio Chapter

CHAIR	Mohan Sankaran, Case Western Reserve University
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Ernest B. Yeager Award

In 1962, the Cleveland Section of the Society for Applied Spectroscopy established the Ernest B. Yeager Award, which now consists of a certificate and a three hundred dollar stipend. This award is made annually to an outstanding undergraduate student who is attending a college or university in Northeastern Ohio, and who has demonstrated an interest in some phase of spectroscopy. The award also carries a free one-year membership in the Society for Applied Spectroscopy.

Year	Recipient	Year	Recipient
1962	Eric A. Entemann	1990	No Award Given
1963	John H. Konnert	1991	Stephen C. Stone
1964	Sheldon J. Green	1992	No Award Given
1965	Cheryl H. Miller	1993	Baonian Hu
1966	Dale Wingeleth	1994	Amy L. Lusk
1967	Richard D. Ash, Jr.	1995	John W. Cave
1968	Jon Mynderse	1996	Michael Fiorentino
1969	Virginia E. Coates	1997	Jonathan Flad
1970	Charles F. Cobb	1998	Christopher S. Callam
1971	Gerald R. Cappo	1999	David T. Clark
1972	Donald R. Diehl	2000	Adam Van Wynsberghe
1973	Fred A. Fortunato	2001	David C. Oertel
1974	Douglas B. Rahrig	2002	Richard L. Barger, Jr.
1975	William Hart	2003	Michelle Adams
1976	John Havens	2004	Tiffany Leigh Copeland
1977	Thomas M. Leiden	2005	Stacey Lynne Dean
1978	Scott A. Raybuck	2006	Colleen M. Burkett
1979	Jeff Weidenhamer	2007	Manasi Bhate
1980	Alexander Kondow	2008	Nikolas Joseph Neric
1981	Raymond E. Cline	2009	Deacon J. Nemchick
1982	Marie Zaper	2010	Rachel V. Bennett
1983	Brian L. Cousins	2011	Daphne A. Guinn and Jennifer L. Miller
1984	Ka-Pi Hoh	2012	Jean Quenneville
1985	Chris Scott	2013	Yihui Chen
1986	Ann M. Mulichak	2014	Jocienne Nelson
1987	Rex Ramsier	2015	Kevin Budge
1988	Joy Gorecki	2016	Ian Campbell
1989	Sheryl Tucker		

2017 Ernest B. Yeager Award Recipient

Rachel Molé
The College of Wooster

“Assessing Load Reduction of Pharmaceutical Compounds in Effluent Post-Disinfection at Chicago’s O’Brien (UV) and Calumet (ClO⁻) Water Reclamation Plants: HPLC-MS/MS Analysis of Effluent Combined with Bench- Scale Simulations”

Ernest B. Yeager, the Frank Hovorka Professor Emeritus of Chemistry at Case Western Reserve University, was internationally known for his pioneering contributions to the fundamental understanding of electrochemical reactions and to the development of fuel cell and battery technology. During nearly 50 years on the Case Western Reserve faculty, he mentored 80 doctorate students and 45 post-doctorate fellows, authored 270 scientific papers and edited and co-edited 20 books. He was internationally recognized as an authority in physical acoustics and electrochemistry. His students and colleagues knew him for his uncompromising demand for excellence in research and scholarly writing. Professor Yeager, 77, died March 8, 2002 in Cleveland, Ohio, after a long struggle with Parkinson’s Disease.

John Bell Memorial Award

John Bell was a long-time member of the Society for Applied Spectroscopy (SAS). The Northeastern Ohio Science and Engineering Fair was one of John's special interests; he took great pleasure in representing our Society's local section as a judge at this event. Unfortunately, John died in November 1994. After his death, the members of the Cleveland Section of SAS voted to honor him by establishing the *John Bell Memorial Award*, for the Science Fair project which best uses or illustrates a principle of spectroscopy in an innovative manner.

Year	John Bell Award	John Bell Merit Award	Special Mention Award
1995	Mary Elizabeth Bruce		
1996	Jonathan Parkhurst		
1997	Lavanya Kondapalli		
1998	Justine Wang	Vivek Mathur	
1999	Elizabeth Long	Kara Urbanek	
2000	Elizabeth Wood	Srinivas Kondapalli Frank Pucci	
2001	Catherine T. Burke		
2002	Mallory Horejjs	Alia Evans Monica Sberna	Gabe Jakubisin Scott Brigeman
2003	Zenon Mural	Cecilia Michel Monica Benedikt	Matthew McPheeters Christina Beall
2004	Kevin Rinz	Emily C. Wirtz Sarah Lynn Martin	Gabrielle L. Petrie Zack Puskar
2005	Christine Debaz	Simone Duval Sara Yacyshyn	
2006	Ellen Napoli	Patrick Rinz Julia Juster	Brittney Williams Derek Poindexter
2007	Anna Faist	Mary Ryan Jennifer Haag	Rebecca Rabinovich Margarat Sivit
2008	Jonathan Sender	Shrey Shah Johnathan Ungvarsky	Daniel Kernan Peter Suwondo
2009	Katherine Reading	Johnathan Ungvarsky Morde Khaimov	Daniel Krentz
2010	Maddie Mooney	Katrina Feldkamp	Samuel Stroebel Leat Perez
2011	Kevin Yang	Emily Peterson	Sara Mann Jane Kim
2012	Jane Kim	Dongham Kim Maurice Ware	Paige Rogozinski Noah Nicholas
2013	Grace Gamble	Justin Boes	
2014	Alison Jin	Claire Chalkin Anjali Prabhakaran	Morgan Fink Kenna Marblestone
2015	Christine Larson	Nicholas Kernan	Lauren Zipp Ian Thompson
2016	Klaudia Sirk	Adriana Gildone	Audrey Higgins Kei Kojima

The 2017 John Bell Memorial Award Recipient

Maya Dori

“Measuring the Speed of Light with a Microwave Oven”

The 2017 John Bell Memorial Merit Award Recipient

Natalie Haddad

“Got Milk? Mapping the Zinc Concentration in Homemade vs. Silk Almond Milk”

The 2017 John Bell Memorial Special Mention Award

Patrick McFarland

“Supra Macromolecular Cages Self-Assembled by Terpyridine Based Ligands”

**Poster Session
Biological Sciences Section**

Samuel Bunting UAKron Dept. of Chemistry	Measuring Bacterial Growth Using a 3D-Printable Spectrometer
Haidong Zhu UAKron Dept. of Polym. Sci.	Synthesis of Biodegradable Silicone Functionalized Polyester Scaffolds for Bone Tissue Engineering
Krishna Ojha UAKron Dept. of Chemistry	Dependence of Bacterial Cell Respiration on Membrane Fluidity
Daniel Morris UAKron Dept. of Chemistry	Acrylamide Warheads for Targeted Drug Design against Bacterial Glutaredoxins
Weizhuan He LCCC Dept. of Biology	Obtaining a CCR5 Knockout Using the CRISPR/Cas9 System
Doug Rohde Lake County Crime Lab	Postmortem Tissue Distribution of AB-CHMINACA Following Lethal Intoxication Compared with AB-CHMINACA Concentrations in Impaired Drivers
Qing Wang UAKron Dept. Chem. & Biomol. Eng.	Prolong the Release of a Hydrophilic Drug by Incorporating Octadecyltrichlorosilane to Alginate Microcarriers
Eddie Jackson LCCC Dept. of Biology	The Effects of Nitrogen Limitation on <i>Planktothrix agardhii</i>

Physical Sciences Section

Siddhesh Dalvi UAKron Dept. of Polym. Sci.	Direct Evidence of Unsaturated Carbon Formed Using Plasma Polymerization
Haifeng Qin UAKron Dept. of Chem. Eng.	Characteristics and Tribological Performance of an Ultra-durable B4C/Cr Coating with pre-UNSM Treatment
Heather Ketchum LCCC Dept. of Chemistry	GC-MS Analysis of Chinese Baijiu Spirit Flavored as American Whiskey
Janet Gbur CWRU Dept. Mat. Sci. & Eng.	Characterizing Inclusions in Superelastic Nitinol Fine Wires
Mohammad Umar Farooq Khan UAKron Akron Eng. Res. Ctr.	Advanced Spectroscopic Techniques for Studying the Passivation Characteristics of Cr and Na ₂ CrO ₄ Containing Al
Mohamed ElKabbash CWRU Dept. of Physics	Tunable Omnidirectional Light Absorption in Meso-porous Silica Capsules Embedding Plasmonic NPs
Greta Cukrov Kent State Liq. Crystal Instit.	Dynamic Surface Topography of Liquid Crystalline Polymeric Coatings with Predesigned Topological Defects
Michael Delancy Shimadzu Sci. Inst.	ONE SHOT XRD Analysis Using a Wide-Range High-Speed Detector

Keynote Address

“Cyanobacterial blooms in Lake Erie – is there ANY good news?”

George S Bullerjahn
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Toxic cyanobacterial blooms have increasingly plagued western Lake Erie and its embayments for the past twenty years. The complete shutdown of the Toledo water system in 2014 due to microcystin contamination has led to a statewide effort to understand bloom composition, growth characteristics and sources of nutrients. Subsequently, this information will inform models that help set policies that can mitigate bloom events. This talk will discuss the properties of current harmful cyanobacterial taxa along with the measures that are necessary to detect, monitor and ultimately reduce the extent of future blooms.

Presentation IA-1 (Invited)

Sensory, Motor, System: Creating a Replacement Sensorimotor System for Prosthetics

Dustin J. Tyler, PhD
Kent H. Smith Professor, Biomedical Engineering
Case Western Reserve University., Dept. of Biomedical Engineering
Cleveland VA Medical Center
Cleveland, OH, USA

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There are more than 1.6 million people in the United States living with missing limbs. When missing a limb, the *loss of function is detrimental*, but the *loss of sensation is devastating* - somatosensation is one's most significant connection to the world and others. Prosthetics are robots intended to replace the lost limb. To be fully successful as a limb replacement, the prosthetic needs to be embodied, i.e. perceived as integrated into one's body image. This requires 1) agency – control of the actions of the limb, 2) visual-tactile integration, and 3) the integration of motor and sensory systems for naturalistic touch and movement. Traditional prosthetics have not achieved this goal because their connection to the human does not directly interact with user's the motor and sensory system. To overcome this limitation, we have implanted interfaces directly in the muscles and nerves in the remaining limb of the user. This creates a direct link to the user's neuromuscular system. When the user naturally moves their phantom hand, i.e. just thinks about moving their hand, we can reproduce 4 naturalistic degrees of freedom in the prosthetic system that mimic the user's intended motion. Sensors on the prosthetic hand record the interactions of the prosthesis with objects. The sensor data is converted to stimulation of the nerves in the subject's arm. The subject feels all the sensation directly in their hand. They feel *their hand*, not the prosthesis, touching and manipulating objects. This is a significant advance for people with limb loss, but more importantly demonstrates a new level of connection between the persons and machines. There is wide-ranging potential for expanding virtual and mixed reality systems to usher forth a new revolution in man's potential and capability.

Presentation IA-2

Characterizing Impact Damage of Ceramic Matrix Composites using Micro-Computed Tomography and Optical Microscopy

Michael J. Presby and Gregory N. Morscher
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The implementation of the first components made from ceramic matrix composites (CMCs) in jet engines has led to improved engine efficiency and increased propulsion. Compared to their Ni-based super-alloy counterparts, CMCs are approximately one-third the density, and they can withstand higher operating temperatures without the need to be cooled. While CMCs are first limited to static applications, such as high pressure shrouds, they are ultimately targeted for use in rotating parts, such as turbine blades. Extending CMCs to rotating parts will provide further increases in engine performance and efficiency. In spite of possessing many beneficial properties, such as high strength-to-weight ratio, and high temperature capability, CMCs are intrinsically brittle. The intrinsic brittleness of CMCs exposes concern over their ability to withstand impact by foreign objects. Foreign object damage (FOD) is of great concern because particles ingested into engines can severely degrade and/or cause catastrophic failure to the affect components and/or engine. For the aforementioned reasons, understanding how CMCs behave under impact is critical to improving their impact resistance for use in jet engines. The impact resistance of 2-D and 3-D fiber architectures are explored by impacting the specimens at 350 m/s using 1.59mm projectiles. Furthermore, several curved specimens are impacted to determine the impact resistance of more complex geometries which will arise from incorporating CMCs from static to rotating components. Micro-computed tomography (μ CT) and optical microscopy were utilized to provide insight on how the impact damage propagates and interacts with the constitutive components of CMCs.

Presentation IA-3

Atom Probe Tomography: Technology and Applications

Daniel F. Lawrence
CAMECA Instruments, Inc.
5500 Nobel Drive
Madison, WI 53711

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Atom Probe Tomography (APT) provides nanoscale chemical characterization in 3D. In many cases, APT results resemble the best qualities of both TEM/STEM and SIMS combined, with powerful images and seemingly infinite elemental analysis capabilities, including the investigation of buried interfaces, profiles across features, sub-volume composition analysis, and cluster analysis, to name a few. A technology review will be provided to explain the operating principle of the APT instrument as well as a look at sample preparation and the data reduction process. Additionally, a number of analyses will be reviewed in depth and will include a sampling from the rapidly expanding set of proven Atom Probe Tomography applications.

Presentation IA-4

Cryo-Electron Microscopy Reveals an Anthrax Pore Intermediate

Harry Scott¹, Derek Taylor¹ and Jim Bann²

¹Case Western Reserve University, Department of Pharmacology
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Cleveland, OH 44106

²Wichita State University, Department of Chemistry

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Pore-forming toxins are secreted by several bacterial species and provide a strategic advantage to the bacteria that produce these toxins. The anthrax bacteria (*Bacillus anthracis*) secretes a tripartite toxin system that is cytotoxic to the infected host cell which is partially due to its ability to inhibit the host's endogenous defense mechanisms. The scaffold and delivery component of the tripartite toxin system, protective antigen (PA), is secreted by the bacteria and forms a heptameric prepore that presents a binding platform for the toxins, lethal factor (LF) and edema factor (EF). Binding of PA to the capillary morphogenesis gene-2 and tumor endothelial marker-8 receptors, along with proteolytic cleavage and oligomerization, facilitates the assembly of the tripartite toxin system on the extracellular surface of the cell membrane of the infected host. Once assembled, the PA-LF/PA-EF prepore complex is endocytosed whereby the acidic environment of the late endosome triggers a pH-induced conformational change of the prepore complex. This structural rearrangement drives maturation to a distinct membrane-spanning pore that is necessary for delivery of EF and LF to the cytoplasm of the infected cell. We have expressed a mutant PA protein (D425A) that blocks pore-formation by trapping the PA prepore in a novel, intermediate and benign state. We are using cryo-electron microscopy to solve the three-dimensional structure of the stalled anthrax pore-intermediate. This structure will be used to understand anthrax pore maturation and will be useful in the design of small molecule inhibitors designed to block pore formation to prevent anthrax induced cytotoxicity.

Presentation IB-1 (Invited)

Minority and Majority Currents in Doped Organic Field-Effect Transistors

Shiyi Liu, Akram Al-Shadeedi, Vikash Kaphle, Chang-Min Keum, and [Biörn Lüssem](#)

Kent State University
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Organic field-effect transistors (OFETs) have the potential to become the basic building block of a flexible electronics technology used e.g. in flexible displays or wearable sensor systems. Doping these transistors can make them not only more reliable and reproducible [Applied Physics Letters **104**, 013507 (2014)], but opens a new perspective on OFETs. For the first time, generation and dynamics of minority and majority currents can be studied in lightly doped films [ACS Appl. Mater. Interfaces **8**, 32432 (2016), Nature communications **4**, 2275 (2013)].

In this presentation, our current understanding of doped OFETs will be discussed [Chem. Rev. **116**, 13714 (2016)]. An emphasis will be placed on p- and n-doped pentacene-based OFETs, and a new model to describe generation of minority charge carriers inside pentacene will be proposed. Furthermore, the working mechanism of an organic depletion type transistor – the organic electrochemical transistor – will be presented and strategies to optimize their performance will be proposed [Advanced Materials Volume **28**, 8766 (2016)].

Presentation IB-2

Synthesis and Characterization of Pulse Reverse Current Based Electrodeposited Ni-W Coatings

Devesh Dadhich Shreeram^{1,2}, V. Bedekar², S. Enbothula^{1,2}, G. L. Doll^{1,2}

¹Department of Chemical and Biomolecular Engineering

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²Timken Engineered Surface Laboratories

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The need for coatings with both high corrosion and wear resistance remains unmet. Although electrodeposited coatings can have excellent corrosion resistance, their wear resistance is inadequate for many applications. On the other hand, vacuum deposited coatings can provide excellent wear resistance, but tend to have very poor corrosion resistance. This study reports the results of Taguchi Designed Experiments used to derive and optimize parameters for the deposition of Ni-W coatings by pulsed reverse current electrodeposition method. Physical properties of the coatings were examined by SEM, XRD, XPS, XEDS and nanoindentation. Additionally, TEM-based orientation mapping was performed on the Ni-W coatings for orientation and grain size analysis. The corrosion performance was evaluated using EIS and Tafel in 3.5% NaCl solution. The tribological studies were performed in fully formulated and additive-free oils. The tribological and corrosion performances of the coatings were finally compared to the baseline and an industrial standard coating tested in similar conditions.

Presentation IB-3

One-Pot in-situ Preparation of Polypyrrole Composites with Metal Oxide Fillers

Veronica Livingstone and Cora Lind-Kovacs
University of Toledo
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Pyrroles consist of a five-membered ring containing a nitrogen atom, which can be polymerized to form long polymer chains. These polypyrrole chains have a wide variety of applications with two primary functions: sensors and electronics. To improve the properties of pristine polypyrrole, composites will be formed with molybdenum oxide (MoO_x) to improve conductivity, thermal, and mechanical stability. It is especially advantageous to use MoO_x nanoparticles, which fit seamlessly into the composite and have high surface area, allowing for more intimate interactions with the polymer. MoO_x is an ideal choice for use in a composite because it is inexpensive, electrochemically active, and can be crystallized at low temperatures. Composite formation is usually a multi-step process that must be carefully optimized. To increase the efficiency of the production process and optimize the homogeneity of these polypyrrole/MoO_x composites, we are developing a one-pot in-situ process that uses compatible reaction conditions for the simultaneous formation of MoO_x and polypyrrole. Materials are characterized by PXRD, FTIR, SEM, EDS, and MALDI-MS.

Presentation IB-4

Synthesis and Characterization of $A_xSc_{2-x}Mo_3O_{12}$ using non-Hydrolytic Sol-Gel Methods

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Most materials show positive thermal expansion (PTE) and have been highly studied. However, recently, negative thermal expansion (NTE) materials have been of great interest because of their unique properties and potential to tune expansion of composites. Here we study NTE materials in the $A_2M_3O_{12}$ family (A = trivalent cation, M = Mo, W). For some of these materials a temperature dependent phase transition from an orthorhombic to a monoclinic crystal structure has been observed, where only the orthorhombic phase shows NTE. Of interest are the factors that affect monoclinic to orthorhombic phase transitions of these materials and to determine at what temperatures they occur. Trends have been observed for some of these materials, but these trends do not explain the properties of all NTE materials. For example, $AlScMo_3O_{12}$ shows a much lower transition temperature than either $Al_2Mo_3O_{12}$ or $Sc_2Mo_3O_{12}$. Further exploration is necessary to expand the knowledge necessary to tailor these materials to exhibit specific properties for use in composites. The goal of this research is to synthesize novel $A_2M_3O_{12}$ mixed A-site occupancy materials using non-hydrolytic sol-gel methods and investigate their phase transition behavior as a function of composition. Non-hydrolytic sol-gel methods allow for an increase in homogeneity as well as lower synthesis temperatures. Various $A_xSc_{2-x}Mo_3O_{12}$ compounds have been synthesized using non-hydrolytic sol-gel methods, and their characterization is presented in this work.

Presentation IC-1 (Invited)

Tracking Organelles in the Visual System: Insight into Mechanisms of Glaucoma

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Glaucoma, the major cause of irreversible blindness, is a neurodegenerative disease that leads to death of retinal projection neurons, the retinal ganglion cells. The mechanism of degeneration appears to be compartment-specific in that the axon degenerates prior to the cell body. Our investigation of the axon degeneration indicates that retinal ganglion cells suffer from a metabolic dysfunction that may have its origin in the mitochondria. We analyzed mitochondria by transmission electron microscopy and serial scanning electron microscopy, finding evidence for a lack of mitochondrial recycling (“mitophagy”) in the ganglion cell axons. We then turned our attention to mitophagy-associated organelles, quantifying them in both proximal and distal optic nerve. There were significantly greater numbers of autophagic vesicles in glaucomatous optic nerve compared to control. Within glaucomatous optic nerve, there were significantly greater numbers of autophagic vesicles in optic nerves where deficiencies in anterograde axon transport were observed. Distribution of specific organelles such as endosomes, lysosomes, and autophagosomes were significantly altered in the glaucomatous optic nerve. These data suggest that autophagy initiation occurs in the retinal ganglion cell axons in glaucoma, though it may be insufficient to address accumulated proteins and organelles that require degradation.

Presentation IC-2

Role of the Crimpy-Gbb Signaling Pathway at Synapses

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The bone morphogenic protein (BMP) pathway directs growth and neurotransmitter release at the *Drosophila* neuromuscular junction (NMJ). Distinct pools of the BMP ligand Glass bottom boat (Gbb) control NMJ structure and function. While postsynaptic Gbb promotes overall NMJ expansion, presynaptic Gbb promotes neurotransmission. Through our discovery of the neuronal transmembrane protein Crimpy, we were able to identify the presynaptic pool of Gbb. We found that Crimpy delivers neuronal Gbb to dense core vesicles (DCVs) for activity-dependent release. Upon DCV exocytosis, both a Crimpy C-terminal fragment and Gbb are released from terminals, defining an activity-dependent presynaptic signal.

Currently, we are defining the role of the activity-dependent Gbb signal in synaptic assembly, maintenance, and function. To characterize the separate pools of Gbb, I created mutants lacking the presynaptic Gbb signal called "Gbb muscle rescue." Using high-resolution STED microscopy, we find that these mutants display aberrant presynaptic organization at a relatively late developmental stage. Presynaptic defects in these mutants are also observed in electron microscopy ultrastructural analyses. Moreover, the orderly apposition of presynaptic release sites and postsynaptic receptor fields is disrupted. The synaptic defects observed at these late developmental stages raise the question of whether Gbb is only required for maintenance of synapses or whether it is also required for initial synapse assembly. Presently, we are determining if presynaptic Gbb is necessary for the assembly of synaptic components. Analysis of synapse formation in embryos lacking either pre- or postsynaptic Gbb will establish if these signals contribute to initial NMJ synaptogenesis at the NMJ.

Presentation IC-3

Quantification and Characterization of Coronary Collateral Arteries using Micro-Computerized Tomography (CT)

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Coronary collateral arteries are small vessels that interconnect two coronary arteries. In a healthy human heart, these collateral arteries remain small and unused. However, in a disease such as a heart attack, a major artery may become blocked. In these cases, any native collaterals and newly formed collaterals can reach the infarct area ensuring there is sufficient blood and nutrients. We are studying the presence of pre-existing and the growth of new collaterals in mice. We have three test groups: control (healthy, normal), myocardial infarction (MI), and repetitive ischemia (RI). In the MI group, the left descending artery (LAD) is completely blocked by permanent ligation, modeling a major heart attack. In the RI group, a balloon is placed over the LAD. The balloon is periodically inflated, occluding the LAD, and then deflated. This is a model for short repeat episodes of ischemia. In each group, the mice are sacrificed, the hearts are perfused with Microfil, a contrasting compound, and scanned using micro-computerized tomography (CT) at high resolutions (4-8 μ m). The CT images are then analyzed using the 3D analyzing software, Avizo, to qualitatively view the collaterals, and Analyze 12.0 to quantitatively analyze the vessels. We hypothesize that when the heart is under stimulation, new collaterals will grow to provide blood and nutrients to the damaged area. Our analyses support the concept that mice do not possess appreciable native coronary collaterals, but in the event of insufficient blood flow, there is robust formation of collaterals.

Presentation IC-4

Capture of Mycobacterium Smegmatis mc(2)155 on Alumina and Silica Substrates of Various Surface Potentials

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Pulmonary tuberculosis causes more than 1.5 million deaths annually. Smear microscopy is a primary detection tool in areas where 95 % of cases occur. This technique, in which the sputum of a patient is examined using light microscopy for Mycobacterium tuberculosis shows sensitivity between 20 and 60 %. Insufficient mycobacterial isolation during sample preparation may be a reason for low sensitivity. We tested the influence of surface potential on capture of the non-pathogenic model M. smegmatis with the goal of beginning to design a system to more efficiently isolate mycobacteria from suspension on the basis of electrostatic interactions, to increase sensitivity of concentrated smear microscopy. Silica (SiO₂) supports with positive surface potential, coated with polycation, poly(diallyldimethylammonium chloride) (pDADMAC), captured approximately 12.8 times more Mycobacterium smegmatis than SiO₂ substrates with negative surface potential. Compared to smears of M. smegmatis, pDADMAC-coated SiO₂ captured nearly an order of magnitude greater mycobacteria, implying that a lower limit of detection may be achievable with such a system. In this preliminary work, we probe the influence of electrostatic interactions on M. smegmatis capture to inform our design of a capture system for integration into concentrated smear microscopy procedures, requiring minimal extra resources and training for implementation in areas of need.

Yeager Award Presentation

Assessing Load Reduction of Pharmaceutical Compounds in Effluent Post-Disinfection at Chicago's O'Brien (UV) and Calumet (ClO⁻) Water Reclamation Plants: HPLC-MS/MS Analysis of Effluent Combined with Bench-Scale Simulations

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Over the past two years, funding from the National Science Foundation has allowed a team of chemists and biologists to study the effect of newly installed disinfection systems in wastewater treatment at the O'Brien and Calumet plants on reducing the concentrations of estrogenic, androgenic and neuro-endocrine pharmaceutical compounds. It was hypothesized that disinfection would aid in degradation pharmaceutical compounds. The study was designed to help plant operators understand the benefits of UV and/or chlorination disinfection on treating contaminants of emerging concern and provide data on which process is most effective at reducing pharmaceutical loads. Bench-scale testing was performed using either UV or chlorination treatment to validate the transformation of these pharmaceutical compounds. Statistically significant decreases in the concentration of some pharmaceutical compounds were observed in effluent collected pre- and post-treatment. Decreases matched the bench-scale studies. Overall, UV photochemistry and chlorination has shown to be able to transform estrogenic and neuro-endocrine disrupting compounds and may be a side-benefit to disinfection. This presentation will emphasize UV photochemistry results and HPLC-MS/MS used to measure sub-ppb levels of drugs in complex matrixes.

Poster Number One

Measuring Bacterial Growth Using a 3D-Printable Spectrometer

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Visible light spectroscopy is a commonly used technique for measuring the growth of bacterial cultures, and growth curves provide broadly important data. However, the equipment and resources required for these experiments has been restricted to higher education and industry due to high cost and sophistication. We have previously reported on an inexpensive, 3D-printable photospectrometer called the SpecPhone. This device utilizes an iPhone as the camera, along with several other, inexpensive additions to make a fully functional spectrometer. Here, the application of the SpecPhone is expanded to the quantification of actively dividing *E. coli* cultures. Two protocols are described; one describes a culture grown in a beaker and the second is a downsized culture grown entirely in a plastic cuvette. These protocols provide hands-on teaching opportunities for the use of spectroscopy to measure bacterial growth, and to do so in educational situations that may have been previously excluded.

Poster Number Two

Synthesis of Biodegradable Silicon Functionalized Polyester Scaffolds for Bone Tissue Engineering

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Tissue engineering technology uses the combination of cells, materials and engineering methods, and suitable biochemical and physicochemical factors to improve or replace biological functions. Scaffolds are frequently involved in tissue engineering. Scaffolds are biodegradable materials that have been modified to form new functional tissues for medical purposes. Many studies indicated that silicon is an essential element in bone and connective tissue formation. By functionalizing the biodegradable poly(lactic acid) with silicon, its application in tissue engineering is available. The silicon-functionalized copolymer used in this study was synthesized by grafting methyl methacrylate and a silicon-containing methacrylate by atom transfer radical polymerization (ATRP) from a brominated poly(lactic acid) (PLB) used as a macroinitiator. The PLB macroinitiator (GPCPSt $\bar{M}_n = 1.6 \times 10^4$ Da; $\bar{D} = 2.25$) was prepared by incorporating 2-bromo-3-hydroxypropionic acid (BrH) as a co-monomer with lactic acid (LA). This polymerization was well controlled using CuBr as the catalyst and bipyridine as the ligand in toluene at 90 °C. The resulting graft copolymer contains PLA, PMMA and 3-(triethoxysilyl)propyl methacrylate (TESPMA). The final scaffolds prepared by compression method showed good integrity in cell culture media.

Poster Number Three

Dependence of Bacterial Cell Respiration on Membrane Fluidity

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Electron Transport Chain (ETC) is used to generate the energy through the multiple redox reactions during cellular respiration where oxidation of sugar molecules generates ATP via proton pumping across a membrane from cytoplasm to periplasm. Normally, electrons are transported through the membrane soluble electron carrier ubiquinone. It is proposed that the ETC activity of the cell is related to the membrane fluidity because of the diffusion of ubiquinone. To analyze this phenomenon, membrane fluidity and cell respiration measurements will be performed on the same single cells. Fluorescence Recovery After Photobleaching (FRAP) technique is used to determine the fluidity of membrane components. Cell respiration measurements in bacteria are carried out by measuring the consumption of oxygen by *Escherichia coli*. Redox sensitive dyes are used to look at ETC activity.

Poster Number Four

Acrylamide Warheads for Targeted Drug Design Against Bacterial Glutaredoxins

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Glutaredoxins (GRX) play an integral role in buffering the redox state of cells and are considered mediators of cell processes that occur at specific redox potentials. Acting as a control switch for multiple pathways, GRXs represent an untapped reservoir of novel therapeutic targets. Their dithiol containing active sites are appealing for chemical modification where covalent alkylation of enzymatically important cysteines have already been explored to produce irreversible inhibitors. Cys alkylation is achieved by bringing a vinyl containing functional group into close proximity with the thiol-containing residue. Small vinyl containing compounds alone are highly reactive, nonspecific, and toxic. It is, therefore, necessary to functionalize larger molecules with a vinyl moiety to act as a driving group and facilitate targeted inhibition. Such vinyl containing compounds have been termed “acrylamide warheads.” Variances in surface structure among orthologous GRXs were probed for binding pockets that are species selective for compounds that have the potential to serve as driving groups. Using saturation transfer difference and 2D proton-nitrogen coupled nuclear magnetic resonance spectroscopy, we screened a small molecule library to find fragment compounds that are selective for the GRXs of two common infectious bacteria: *Pseudomonas aeruginosa* and *Brucella melitensis*. To reveal the selectivity of fragments at this early stage they were coupled with acrylamide to produce warhead-like precursors. These compounds exhibited enhanced reactivity with bacterial GRXs vs the human ortholog. Serving as lead compounds, these warhead functionalized fragments could be chemically extended to produce more drug-like molecules.

Poster Number Five

Obtaining a CCR5 Knockout Using the CRISPR/Cas9 System

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Some survivors of the Black Plague, caused by *Yersenia pestis*, have a selective advantage in that they lack a functional *ccr5* gene. A 32 base pair deletion mutation, delta 32, confers resistance to *Yersenia pestis* and HIV infection. Timothy Ray Brown, the only known person to be cured of HIV, received a bone marrow transplant from a donor who was homozygous for the *ccr5* delta 32 mutation. A possible cure for HIV might be the down modulation of CCR5. It has been hypothesized that the amino-terminus of the CCR5 delta 32 protein is capable of exerting a negative regulatory effect on wild type CCR5 as well as CXCR4, an additional secondary co-receptor. This study was designed to determine the effect of the complete removal of the *ccr5* gene in human cells.

Gene editing was performed using the CRISPR/Cas9 system to eliminate the expression of the CCR5 protein by removing a section of the sequence from both copies of the *ccr5* gene. The human T cell line H9 was co-transfected with plasmids containing guide RNA sequences that have homology to the amino-terminus of the *ccr5* gene along with a plasmid containing the CRISPR/Cas9 gene. Puromycin toxicity was determined by serial diluting puromycin into culture medium and counting cells. Stable transformants were obtained by puromycin selection. The presence of the gene in transfected cells was confirmed by PCR of the puromycin gene. The successful ablation of CCR5 will be confirmed and used to test expression of both CCR5 and CXCR4.

Poster Number Six

Postmortem Tissue Distribution of AB-CHMINACA Following Lethal Intoxication Compared with AB-CHMINACA Concentrations in Impaired Drivers

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The appearance of synthetic cannabinoids as recreational drugs began in the US around 2010. AB-CHMINACA, a synthetic cannabinoid, has psychoactive and pharmacological effects similar to delta-9-tetrahydrocannabinol, the active ingredient in marijuana. Comprehensive toxicology and drug chemistry analyses were performed on solid dose and biological samples using gas chromatography / mass spectrometry, ultra performance liquid chromatography / tandem mass spectrometry and high performance liquid chromatography / tandem mass spectrometry in order to identify and quantify AB-CHMINACA.

Poster Number Seven

Prolong the Release of a Hydrophilic Drug by Incorporating Octadecyltrichlorosilane to Alginate Microcarriers

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Hydrogels are excellent drug carriers due to their exceptional biocompatibility, biodegradability and ease of processing. However, they exhibit one intrinsic drawback, its inability to retain drugs, especially hydrophilic drugs, for a prolong period of time, which limits their usage. Sustaining the release of hydrophilic compounds from hydrogel matrices has been actively researched. In this study, a simple approach by incorporating a hydrophobic agent, octadecyltrichlorosilane (OTS), to hydrophilic alginate microspheres (Alg-Ms), the hydrogel drug carrier, was employed to sustain the release of hydrophilic drugs. Sodium benzoate (NaB), a highly water soluble small molecule, was used as the model drug. By increasing the OTS concentration in the solutions used for treating Alg-Ms, the hydrophobicity of the OTS incorporated Alg-Ms, or OTS-Alg-Ms, increased, prolonging the release of NaB. The OTS, fully hydrolyzed, eroded away with the alginate shell when contacting the release medium, but the OTS leached into the medium posed no detectable toxicity towards human fibroblast cells. The release of NaB from these OTS-Alg-Ms was fitted with the Ritger-Peppas and Peppas-Sahlin models and the results showed that NaB released from OTS-Alg-Ms prepared using a solution containing 0.9g/L of OTS was mainly controlled by Fickian diffusion. For OTS-Alg-Ms prepared using a solution having a lower amount of OTS (≤ 0.35 g/L), the microspheres swelled more easily, and the swelling contributed to NaB release. The results demonstrated the simplicity of improving the hydrophobicity of hydrogel drug carriers using hydrophobic molecules, such as OTS, to broaden the drug delivery applications of hydrogels in delivering small hydrophilic drug.

Poster Number Eight

The Effects of Nitrogen Limitation on *Planktothrix agardhii*

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Sandusky Bay has become increasingly plagued with algal blooms over the past few decades due to the surrounding agricultural land usage. Excess nutrients from fertilizers applied to these fields drain into the Sandusky River, which in turn drains into the Sandusky Bay. The shallow waters of the bay, average depth of less than 2m, are insufficient to adequately dilute the nutrients coming from the river. Although nitrogen (N) is rapidly depleted by midsummer in the bay due to sedimentary denitrification, *Planktothrix agardhii* yields a persistent bloom condition, despite the fact that this organism does not fix N (Davis et al. 2015). These blooms affect the aesthetic appearance and water quality of the Bay due high levels of chlorophyll and the production of microcystin, a cyanobacterial hepatotoxin. The Sandusky area depends on the bay as a drinking water source and must take additional actions to preserve potability during blooms. It is suspected that *Planktothrix agardhii* survives N depletion by accessing nitrogen stored in cyanophycin. This N rich polymer, composed of an aspartic acid backbone with arginine branches, is produced by the enzyme cyanophycin synthetase, encoded by the *cphA* gene. During nitrogen limitation, the enzyme cyanophycinase, encoded by the *cphB* gene, hydrolyzes cyanophycin into dimers of aspartic acid and arginine, regenerating nitrogen into central metabolism. In this study, an endemic Sandusky Bay *Planktothrix* strain was grown under N-replete and N-limited conditions to monitor expression of functions associated with N stress. Daily, the cultures were filtered and tested for chlorophyll *a* levels. RNA was extracted and RT-PCR performed to examine patterns of *cphAB* expression.

Davis TW, GS Bullerjahn, T Tuttle, RM McKay and S. Watson (2015) Env. Sci. Technol. 49: 7197-7207.

Poster Number Nine

Direct Evidence of Unsaturated Carbon Formed Using Plasma Polymerization

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Physical and chemical properties of surface/interface are dependent upon the type of chemical functionalities present. Unsaturated carbon (sp² carbon) is an intermediate functionality that is used to modify surfaces for applications in adhesion, friction and wetting. Here we show the evidence of unsaturation on a functionalized polymer surface with the help of contact angle, XPS and Sum Frequency Generation Vibrational Spectroscopy (SFG) techniques. Surface sensitive technique, such as X-Ray Photoelectron Spectroscopy (XPS), probes elemental composition as well as type of functional groups present at first ~10 nm depth of the surface through high resolution scans. Previously, unsaturated carbon has not been confirmed using a high resolution C1s spectrum of a polymer surface. SFG shows the presence of vinyl groups at the interface. Thus the surface vinyl groups are not just characterized qualitatively but also quantitatively. A comparison of vinyl terminated self-assembled monolayer and plasma polymerized acetylene surface shows similarity in chemical composition.

Poster Number Ten

Characteristics and Tribological Performance of an Ultra-durable B4C/Cr Coating with pre-UNSM Treatment

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In this work, B4C/Cr coating was deposited onto AISI 52100 disks with additional C2H2 gas. Ultrasonic nanocrystal surface modification (UNSM) technique was used to pre-treat the samples. UNSM treatment can refine grain sizes, increase hardness, and induce compression residual stress in the near surface region to make the substrate more compatible with the mechanical properties of the coating. Mechanical properties of the coatings were studied by indentation techniques and scratch testing. Microstructural and compositional properties were characterized with Raman spectroscopy, Fourier transformation infrared spectroscopy (FTIR). Tribological performance of the coatings was evaluated on specimens using pin-on-disk (POD) tribometer under dry contact condition. Results show that UNSM treatment enhanced the adhesion of the coating with the AISI 52100 substrate, and by adding C2H2 gas during deposition process, friction coefficient was reduced. Thus, the B4C/Cr coated disks provide a significant improvement on wear resistance.

Poster Number Eleven

GC-MS Analysis of Chinese Baijiu Spirit Flavored as American Whiskey

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Gas Chromatography-Mass Spectroscopy (GC-MS) is routinely used to profile the flavor compounds in alcoholic beverages. This method has been applied to unique experimental samples of Chinese Baijiu liquor flavored to taste more similar to American whiskey. Chinese Baijiu is a clear liquor, usually considered strong in flavor by the western palate. In an effort to modify these liquors into something more akin to the routine western palate, experimental samples have been produced of Chinese Baijiu liquors flavored to taste similar to American bourbon. This has been accomplished by subjecting Chinese Baijiu liquor to a novel accelerated aging process which employs pressure, as opposed to conventional time, to mature the spirit quickly and impart wooden barrel flavors. By processing Chinese Baijiu liquor via this innovative technology of accelerated pressure aging, the clear spirit becomes colored and flavored with wood in the short time of a few days. The distinct flavor compounds in these experimental liquors have been identified and profiled using routine straight injection GC-MS. As such, it has been determined that wood aged Chinese Baijiu spirit flavor is characterized by unbranched aliphatic esters. Foremost, aging Chinese Baijiu in wood increases the concentration of ethyl hexanoate, which imparts a sweet and fruity nuance.

Poster Number Twelve

Characterizing Inclusions in Superelastic Nitinol Fine Wires

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Continued advancement in minimally invasive surgeries coupled with the miniaturization of medical devices places a greater demand on the robustness and reliability of the constituent materials. Enhanced performance requirements of fine wires/strands used as surgical tools or as components of medical devices demand keen attention to material processing. Successful material applications require a strong understanding of the relationship between material composition and processing to the fatigue and fracture behavior. Microscopic material features such as inclusions and voids can contribute to premature failure which may lead to adverse conditions while in use as a tool or as an implanted device. Characterization of these features; therefore, is critical to the overall understanding of the material behavior. In this study, fine wires (<0.200 mm diameter) of superelastic Nitinol were obtained in a standard grade material and a high purity material. The as-received wires were evaluated with various metallographic techniques using longitudinally prepared samples. Correlative microscopy was used to tie conventional bright field microscopy and differential image contrast (DIC) methods to scanning electron microscopy (SEM). To confirm the chemical composition of the matrix, inclusions and/or intermetallic phases, electron dispersive spectroscopy (EDS) and scanning auger microscopy (SAM) were used to provide quantitative elemental analysis and mapping where possible. In addition, specimens were serial sectioned, transversely, with a plasma focused ion beam technique in order to capture the three-dimensionality of the features of interest. Analysis of the inclusions (size, distribution, chemistry) is presented and a comparison of the material grades is discussed.

Poster Number Thirteen

Advanced Spectroscopic Techniques for Studying the Passivation Characteristics of Cr and Na₂CrO₄ Containing Al

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Passivation of aluminum is a beneficial attribute to its electrochemical characteristics; improving its corrosion behavior in various aqueous environments. Characteristics of the passive film play important role in determining the overall corrosion behavior. Breakdown of the passive film leads to the pitting corrosion and limits the application of aluminum in many environments. In the present study, the composition of the passive films developed on Al5at.%Cr alloy and Al x-Na₂CrO₄ was studied. Al5at.%Cr alloy and Al x-Na₂CrO₄ (x=5, 20 wt%) were prepared by high energy ball milling (HEBM) and subsequent consolidation. The microstructure of consolidated samples was studied using scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDX). Al5at.%Cr was polarized at 20 mV above open circuit potential for 30 min in 0.01 M NaCl and subsequently studied using auger electron spectroscopy (AES), which revealed the influence of the microstructure on the evolution of the passive film. Al x-Na₂CrO₄ (Na₂CrO₄ containing aluminium) were immersed in 0.01 M NaCl for 1 h followed by characterization using X-ray photoelectron spectroscopy (XPS) to investigate the chemical composition of the passive film as a function of Na₂CrO₄ content. Composition of the passive film studied using AES and XPS in the two materials was correlated with their corrosion behavior and microstructure.

Poster Number Fourteen

Tunable Omnidirectional Light Absorption in Meso-porous Silica Capsules Embedding Plasmonic NPs

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A major problem facing the proliferation of solar energy generation is energy storage. Although, photovoltaic generators enjoy high efficiency, they suffer from high energy storage costs. Conversely, concentrated solar power plants collect and store heat and dispatch electricity at lower storage costs but with less efficiency. To address these problems, hybrid solar converters were proposed to exploit the high efficiency of photovoltaics and the low costs of solar energy storage. The excess solar energy not used to produce electricity can be stored as heat. A promising class of materials that can convert light to heat efficiently are black metals. Top-down approaches to create black metals offers flexibility of design and control on the absorption range. However, these designs are expensive and time consuming. Bottom-up approaches are easier to up-scale but offer little control on their optical properties. Here, we demonstrate a black metal system based on plasmonic absorption of Au embedded in a meso-scale silica shell. By simply changing the growth of the Au and increasing its size, we show that we can control the broadness of the plasmon resonance which is translated into strong heat generation via the plasmonic photo-thermal effect.

Poster Number Fifteen

Dynamic surface topography of liquid crystalline polymeric coatings with predesigned topological defects

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Liquid crystal polymer networks (LCNs) are currently explored as promising materials to create programmable and adaptive soft mechanical elements and systems [1]. The orientational order of the networks is used to preprogram their mechanical response to stimuli such as temperature and photo-irradiation [1]. In particular, topological defects in the director field can cause mechanical deformations of the free-standing LCN films [2, 3]. In this work, we demonstrate that the predesigned director patterns with topological defects can be used to control a dynamic surface topography of LCN coatings. In these coatings, one surface is rigidly bound to a solid (glass) substrate, while the other is free. The director pattern is created by the recently developed photoalignment method based on plasmonic photomasks [4]. A highly ordered polymeric coating is prepared by photoinitiated free-radical polymerization of a mixture of liquid crystal mono- and diacrylate monomers in the nematic phase [5]. As the temperature of the environment changes, the coating responds by changing the topography of the free surface. The topography change is uniquely determined by the type of topological defects and director gradients preprogrammed during the alignment and polymerization of LCNs. In particular, topological defects of strength one with a pure bend of the director produce hills upon heating, while the defects of the same topological charge with pure splay produce valleys. The effect is fully reversible in the heating-cooling cycles. We relate the underlying mechanism to the local expansion-contraction stresses triggered by the temperature-induced changes of the scalar order parameter [1, 6]. To elucidate the mechanism, we explore the mass transport across the coating and within the plane of the coating. The work was supported by NSF grants DMR-1121288, DMR-1507637.

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Poster Number Sixteen

ONE SHOT XRD Analysis Using a Wide-Range High-Speed Detector

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“OneSight”, a wide-range high-speed detection system (with Mythen 1K by Dectris Ltd.) has a silicon sensor array of 1280 channels and can acquire a diffraction profile of more than 10 degrees angle range without moving the goniometer (ONE SHOT analysis). This is useful for quantitative analysis of small samples and residual stress measurement with high sensitivity and high speed.

Compared with the conventional scintillation detector, OneSight achieves higher-speed measurements due to its sensitivity, which is more than twenty times that of the scintillation detector. In quantitative analysis by X-ray diffraction, where one peak of interest is targeted, it is effective to utilize the "One Shot Mode" in which the detector is fixed using a wide acquisition angle that includes the target peak position.

Presentation IIA-1 (Invited)

Advances in Atomic Force Microscopy (AFM) Based Methods to Characterize Polymer Materials on the Nanoscale

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AFM based characterization methods are uniquely suited to identify and discriminate materials since this microscopy is inherently based on a mechanical interaction between a nanoscale tip and sample. In addition to the commonly recognized topography, AFM is uniquely powerful as a tool to explore simultaneously the material's mechanical, electrical, optical, and magnetic properties. In the area of nanomechanical measurements, which are of particular relevance to polymers and soft materials, an ongoing challenge for these kinds of characterization methods is quantitative measurement of viscoelastic properties.

Recent progress has been achieved with advanced AFM methods to quantitatively measure the storage modulus, loss modulus, and loss tangent of polyolefin containing blends. Dynamic contact methods are applied to measure the properties of polypropylene containing blends showing excellent sensitivity and accuracy in measurements of storage and loss modulus. The loss tangent is also measured as a function of temperature, revealing important polymer transitions. Finally, the use of multifrequency AFM methods, where the AFM cantilever is excited at multiple eigenmodes, is shown to successfully discriminate materials in heterogeneous or multi-component blends and materials.

Presentation IIA-2

Ultrathin Nanometer Scale Absorber Using Lossless Dielectric and Low Conductivity Metal

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The ability to control light in the nanoscale is the cornerstone of modern photonics. One active area of research is to engineer nanostructure that achieve strong to perfect light absorption. These structures have wide range of possible applications in thermo-photovoltaics, solar energy generation, optical filters, electromagnetic shielding and stealth, etc. Using nano-scaled optical coatings present the most promising candidate for practical applications due to its scalability and ease of fabrication. Recently, an ultra-thin nanometer scale absorber was demonstrated using a lossy dielectric and a metal with finite conductivity that can achieve perfect absorption for dielectric thickness $< \lambda/4n$ where λ is the wavelength and n is the dielectric refractive index*. Although this system provides great advantage over other optical absorbers, it is limited to the existence of strong losses in a dielectric which is a difficult condition to achieve over a broad wavelength range. Here, we show that it is possible to achieve critical light absorption in lossless dielectrics with thickness using low conductivity metals as a substrate. Our approach is more practical and flexible as it is not limited to the spectral range where the dielectric is lossy. In addition, it is possible to realize multi-band absorption which is difficult using lossy dielectrics. Furthermore, having a low conductivity metal is advantageous as they usually maintain their low conductivity within a very broad wavelength range that spans the visible and IR ranges.

*Nanometre optical coatings based on strong interference effects in highly absorbing media, Nature Materials, (2012).

Presentation IIA-3

Understanding the Chemical Composition of the *Caulobacter Crescentus* Adhesive Holdfast

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Most synthetic adhesives fail due to poor interfacial adhesion when used in subaqueous conditions. This is due to the characteristic of water in forming a weak boundary layer at the interface, in addition to plasticizing the adhesive. These challenges have been surmounted by natural organisms such as bacteria which thrive in underwater conditions. The bacterium *Caulobacter crescentus* is known to bind strongly underwater by utilizing a discrete adhesive structure called the holdfast. The holdfast exhibits an adhesive strength known to be the highest for any microorganism. Here, we employ Attenuated Total Reflectance Infra-Red Spectroscopy (ATR-IR) to provide a further understanding of the chemical composition of the holdfast adhesive, utilizing a mutant strain of the bacteria on both hydrophobic and hydrophilic surfaces. A comprehensive understanding of the chemistry of the holdfast will bestow the needed tools for translating its characteristics to sustainable, synthetic underwater adhesives with potential applications in medicine, engineering and biomimetics.

Presentation IIA-4

Quantification, Characterization, and Simulation of the Intracytoplasmic Membranes of Methanotrophic Bacteria by Fluorescence Microscopy

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Methanotrophic bacteria have the ability to utilize methane as their sole carbon and energy source. This unique metabolic property makes them an attractive candidate to synthesize potentially useful chemicals, such as biofuels and bioplastics, from a starting material which is both a relatively cheap waste material, and a potent greenhouse gas. To take advantage of this process it is necessary to have an understanding of the intracytoplasmic membrane (ICM) systems in which methane oxidation takes place. These ICM structures have commonly been visualized by transmission electron microscopy (TEM). This technique has significant drawbacks for studying ICM including: long sample preparation, lack of variability in the z direction, and above all the fact that dynamics cannot be observed in TEM samples. To gather more information about in vivo aspects of these membrane systems we use a combination of fluorescence microscopy, as well as coarse grained molecular dynamics simulations. On the microscopy side, we are able to use lipophilic dyes in order to view ICM structures in live cells. These structures can then be quantified under differing conditions or over time to analyze membrane dynamics. Using this technique, we are able to replicate a well-documented copper response in ICM formation, as well as gather other physiologically relevant information by costaining with other dyes of varying properties. On the computational side, we are able to simulate methane partitioning within both single lipid bilayers as well as stacked systems mimicking ICM architecture. These simulations provide us with data regarding changes in partitioning coefficient as well as rate of methane transfer between lipid layers. Adding in enzymes to these simulations is also possible and could in theory lead to discoveries regarding methane's interaction with them during its metabolic journey.

Presentation IIB-1

Analysis of a Novel Mutation Located in the *ccr5* gene with Potential Effects on HIV Infectivity

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To infect a human T cell, HIV must first bind to the CD4 receptor protein, along with one of two co-receptors, CCR5 or CXCR4. In 1995, a missense point mutation in the *ccr5* gene, which encodes for the CCR5 protein, was found in a member of an African-American family. The family consisted of five children who were exposed to the mother's HIV during natural childbirth. Only the second born child did not contract HIV. The mutation, named TG5, was found in the second born child's *ccr5* gene. The mutation occurs at the 314th amino acid and causes a change from lysine to arginine. To determine if the mutation has any effect on the infectivity of HIV, it must first be isolated. Original samples of the mutation were ligated into a pcDNA vector. The sample was digested and ligated into Invitrogen's pCR®4-TOPO® vector, and transformed. The sample was confirmed in the TOPO Vector using PCR techniques. The sample was ligated into the Clontech pLNCX2 retroviral vector. A lipofection was used to transfect PT67 packaging cells with pLNCX2-TG5. The packaging cells will produce retroviral particles which will be purified and used to perform a transduction into H9 cells. Using neomycin selection, cells expressing the TG5 mutation will be isolated. Mutated cells will be tested for HIV infectivity as well as examined to see the effect on the structure of their CCR5 protein. If the mutation has an effect on HIV infectivity, it could potentially be used in future gene therapies.

Presentation IIB-2

Characterizing the Effects of the Delta32 Mutation found from Yersinia Pestis Survivor Descendants on CCR5 Expression and HIV Infectability

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Human Immunodeficiency Virus (HIV) is a virus that can cripple the patient's immune system, rendering it unable to fight it or other infections. HIV must first bind to the primary receptor on the human T-cell, CD4, and one of two secondary receptors, CCR5 or CXCR4, to infect an individual cell. After the HIV glycoprotein 120 successfully binds to the receptors, it uses glycoprotein 41 to pierce and infect the cell. There is a mutation known to affect HIV infectivity. Delta 32 is a deletion mutation of 32 base pairs of the CCR5 human gene sequence. It is theorized that this mutation truncates the CCR5 receptor from the surface of the human T-Cell, making HIV unable to infect human T-Cell. This mutation confers resistance to HIV infectivity as well as Yersinia pestis, when the individual is homozygous.

An individual (subject EN2) who is heterozygous for CCR5 delta32 has been identified. They are a descendent of survivors of a Yersinia pestis outbreak, more commonly known as the Black Plague.

A PCR amplification, from our subject EN2, was performed using primers that circumscribe the CCR5 gene. Both wild type and delta32 alleles were obtained from this individual. These products were then cloned into pCR4-TOPO vector, and will then be excised and cloned into pLNCX2 retroviral expression vector. The retroviral products will be used to create stable and transient transductants into H9 Lymphoid cells and will be tested for HIV infectability and CCR5 expression.

Presentation IIB-3

Carbon Nanotubes Improving Activated Carbon as a Filter Media

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Carbon nanotubes have been grown on activated carbon and evaluated for use as filtration media. A novel process has been developed to grow carbon nanotubes whereby granulated activated carbon (GAC) is infused with catalyst, and carbon nanotubes (CNTs) are then grown with an alcohol precursor. The presence of CNTs was confirmed via SEM imaging and selected samples were further characterized by thermogravimetric analysis (TGA). A Brunauer–Emmett–Teller (BET) surface analysis was performed to compare and contrast GAC versus GAC with CNTs. Samples of activated carbon and activated carbon with nanotubes were evaluated for use as filtration media. Evaluation of the samples as filtration media was performed by testing for removal and recovery of various heavy metals via atomic absorption (AA) spectroscopy. It was thereby determined that the addition of carbon nanotubes to granulated activated carbon improves the filtration of heavy metals for use in industrial settings.

Presentation IIB-4

GC-MS Analysis of Unprecedented Whiskey Flavors Including Chinese Baijiu Flavored as American Bourbon

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Gas Chromatography-Mass Spectroscopy (GC-MS) has been used to profile the flavor compounds in experimental flavors of bourbon which have been produced by a novel accelerated aging process. New unprecedented flavors of whiskey have been generated including cherry, apple, hickory, maple and honey locust, and the distinct flavor compounds in these uniquely flavored bourbons have been identified and profiled. As such, it has been determined that cherry bourbon has an increased concentration of ethyl octanoate, a compound known to impart a sweet fruity flavor, while it has relatively less phenethyl alcohol, a compound known to impart a breadly flavor. Similarly, this method has been applied to experimental samples of Chinese Baijiu liquor flavored as American bourbon, and the distinct flavor compounds identified and profiled. As such, it has been determined that wood aged Chinese Baijiu flavor is characterized by an increase in ethyl hexanoate, which imparts a sweet and fruity nuance.

Presentation IIC-1 (Invited)

X-ray and Neutron Scattering Studies of Confinement Effects in Polymer Thin Films

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X-ray and neutron scattering techniques are playing key roles in elucidating effects of confinement in thin polymer films. X-ray Photon Correlation Spectroscopy, an X-ray analog to dynamic light scattering with visible light, can probe thermally stimulated fluctuations at the surface of a polymer melt film. The dynamics of these fluctuations can be altered very strongly by tethering of polymer chains to a substrate surface and by tethering inside polymers of nonlinear architectures. Gold nanoparticles can be added to the films in order to probe viscosity as a function of depth in the film, using resonance enhancement. Key to understanding the role of the tethering in films containing polymer brushes or only a fraction of chains tethered to the substrate are measurements with neutron reflectivity to define the internal morphology of the film. These various scattering techniques complement one another for probing the effects of interest.

Presentation IIC-2

Crystallite Size Analysis of Nanomaterials by X-ray Diffraction

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Crystallite size determination of nanodiamonds and nano-zincite particles were examined by X-ray diffraction (XRD). Single peak analysis utilizing the Scherrer equation along with whole pattern fitting was carried out. The main focus of this presentation will be to compare and contrast the two different techniques. Peak broadening due to micro-strain often competes with size broadening for larger particles, but adds little effect when crystallite sizes become small (<10 nm), as size becomes the dominant contribution. Williamson-Hall plots were generated for larger particles to separate out the effects of size from strain. XRD data was collected on a Rigaku D/Max 2200 with Cu $k\alpha$ radiation utilizing a nickel filter. Acquired patterns were analyzed with Bruker's DIFFRAC.EVA software. Whole pattern fitting was performed with JADE 2010 from Materials Data Inc. Confirmation of particle sizes was carried out by Energy Filtering Transmission Electron Microscopy (EFTEM) on a Zeiss Libra 200 TEM.

Presentation IIC-3

Study of Solid Solubility and Grain Size of Mechanically Alloyed Al Alloys Utilizing X-Ray Diffraction Analysis

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Aluminum alloys produced by mechanical alloying possess a unique structure that allow them to have exceptional mechanical properties and corrosion resistance. This structure consists of nano-sized grains ($<100\ \mu\text{m}$) and extended solid solubility of the alloying elements. To characterize this structure, X-ray diffraction proved to be a great resource to obtain a quantitative analysis of the chemical composition composition of the matrix, therefore, the extend of the achieved extended solid solubility and the average grain size. The XRD machine was set to Bragg-Brentano mode to account for random crystallite orientation and the grain size was calculated utilizing Scherrer's equation. The atomic fraction of alloying element in solid solution was correlated to previous works where the relationship between lattice parameter and alloying content for sputtered deposited alloys studied. In this work, XRD results from samples produced by mechanical alloying and a literature compilation of the evolution of the lattice parameter of Al alloys with increasing alloying in different Al-M systems produced by sputtering.

Presentation IIC-4

Residual Stress Measurements in Automotive Components via X-Ray Diffraction

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The processing of certain features in automotive components such as crankshafts, gears, shafts, springs, rotors, cylinder heads, engine blocks etc. pose several difficulties for manufacturers and it is often a challenge to produce a finished product with the superior material characteristics that may be required for a given application. Among material characteristics of interest, the residual stress can have a significant impact on the effective service life of a component. Since residual stresses are introduced in nearly every step in manufacturing, it follows that the effect of processing applied to failure-critical locations must be well understood, controlled and optimized. The characterization of residual stresses in automotive components can be performed using the x-ray diffraction (XRD) technique. XRD is often the only viable technique to measure residual stresses at certain failure-critical locations, for example, in the tooth root of a gear. Surface residual stress measurements can be performed nondestructively for inline quality control and for tracking stresses through processing and in-service cycling. Subsurface gradients can also be evaluated for components taken from various stages of manufacture to benchmark subsurface effects of each manufacturing process. Once contributing mechanisms and sources of potentially harmful residual stresses are well understood, fabrication processes can then be modified and optimized so that high quality components can be manufactured at a competitive cost. This presentation will discuss the key aspects of applying XRD to the measurement of residual stress and will cite examples where XRD has been applied to the characterization of some typical automotive components.

Presentation IIIA-1

The Fundamentals of Rheology and the Application in PSA

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Rheology is a very important tool in polymeric industries. Fundamentals of rheology will be introduced in this presentation. Three case studies about how rheology is used in pressure sensitive industry will be shared. The first case study is about the model to connect the performance with structure in PSA. The second case study is about how to use rheology as a tool to screen raw materials. The third case study is about the LAOS rheology can reveal some of the properties that we do not see by linear rheology.

Presentation IIIA-2

Adhesion under Humid Conditions: Lessons from Spider Silk

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Adhesion in humid conditions is a fundamental challenge to both natural and synthetic adhesives. Yet, glue from most spider species becomes stickier as humidity increases. Previous work has shown that spiders use a combination of proteins and hygroscopic salts as adhesive glue. Under humid conditions, the spider glue undergoes a cohesive failure; unlike synthetic adhesives, which fail interfacially. However, it is still unclear how these salts help in tuning the adhesion especially at high humidity. Here, we use a combination of two different spectroscopic techniques, Infrared Spectroscopy and surface sensitive Sum Frequency Generation (SFG) spectroscopy to obtain a molecular level picture of the contact interface for spider capture glue as a function of varying humidity. Experiments are performed with both pristine and washed silk (devoid of hygroscopic salts) to understand the role of salts in these humidity responsive natural adhesives. Correlations between molecular structure and macroscopic mode of failure will be discussed. Understanding spider glue adhesion will help in designing synthetic adhesives that perform well under humid conditions.

Presentation IIIA-3

Liquid Additives for Plastics Injection Molding

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Liquid Additives for Plastics Injection Molding is a discussion of the application of liquid additives used within the injection molding manufacturing process. The most common additives to this process are colorants. The preferred addition point for liquid colorants is at the feed throat of the injection molding machine avoiding waste in the forms of: overproduction of premixed inventories, materials storage, materials losses, handling, and obsolescence. Scientific Molding techniques have been developed to manage molding process variables. The application of practical analysis techniques are required for further the understanding of additive product design. The art, science, and practice of liquid additive manufacturing is reliant upon skilled chemists and specialized tools to manage the variability in additive manufacturing and the impact upon the molding process.

Presentation IIIB-1

Site-Specific Characterization of PEGylated Insulin Isomers by Using Combined Liquid Chromatography and Ion Mobility Mass Spectrometry

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The conjugation of poly(ethylene glycol) (PEG) to protein drugs (PEGylation) has become highly desirable in the biotherapeutics field since it provides many advantages such as increased circulatory half-life, solubility, and shelf-life. The activity of a PEGylated drug depends on the number, size and location of the attached PEG chain(s). Here, a high throughput analytical methodology is demonstrated that ascertains these properties on a PEGylated insulin sample prepared by random amine PEGylation. A combined reverse phase ultra-performance liquid chromatography (RP-UPLC) and ion mobility (IM) mass spectrometry (MS) approach was taken in order to determine the structural properties of the conjugates. Orthogonal hyphenation of RP-UPLC and IM separation methods prior to MS detection allowed a better dispersion along the 2D retention time/drift time (rt/dt) space. In-source dissociation (ISD) was combined with 2D RP-UPLC-IM separation to truncate the conjugated PEG and form intact insulin ions with very short EO chains attached. Several bn fragments were also observed upon ISD. Observation of such bn fragment ions with or without the linker allowed us to determine the conjugation site. Application of the same methodology to the PEGylated A- and B-chain of insulin obtained after disulfide bond cleavage improved the extent of ISD fragmentation, forming almost complete series of bn and yn fragments without the linker in addition to some bn and/or yn fragments that had the linker attached. The presence or absence of these fragments was used to determine each PEGylation site and corroborate the conclusions drawn before disulfide bond cleavage.

Presentation IIIB-2

MALDI-MS/MS to Determine Sequencing Information of Novel Side Chain Liquid Crystalline Copolymers

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MALDI-MS/MS was used to characterize novel side chain liquid crystalline (SCLC) copolymers, which have applications in data storage, sensing and transistors. Fragmentation studies were done to discern the category of the copolymer (e.g. block, tapered, alternating, etc.). MALDI-MS/MS was the most useful analytical technique for this analysis because sequencing information can be achieved from the generated fragments. Acquiring more information about how the copolymer microstructure affects fluidity and length of stability can give insight into its optical properties.

The SCLC copolymer contained two propylene oxide monomer units, each functionalized with a different substituent on the side chain (repeat units A and B); tert-butoxy and H were the initiating and terminating groups, respectively. Useful backbone cleavages were induced utilizing the LIFT method and led to sequence determination by a “bottom-up” approach. Analysis indicated that an ABBABB motif of the two SCLC repeat units was present. This conclusion was reached because the initiating tert-butoxy group was only found in monomeric and dimeric AB fragments, while the hydrogen terminating group was found only in BB fragments. Further, one backbone fragment without end groups and the AB₂ composition was observed (BBA or BAB or ABB). Only the ABBABB sequence reconciled all these observations.

Presentation IIIB-3

Using Infrared and Raman Microscopy to Correlate Visual Images to Chemical Composition

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Vibrational microscopy is a powerful analytical tool that allows for chemical information to be correlated to visual differences in a material. On a micrometer level, infrared and Raman microscopy are most commonly used to probe a wide range of materials from multicomponent polymer films to geological aggregates. Since the two techniques complement each other (e.g. symmetric or asymmetric chemical vibrations), when combined, they offer a holistic vibrational insight to better understand a material's composition, morphology, and/or physical stress. This presentation will focus on how confocal Raman and infrared microscopy can elucidate chemical composition where defects occur, and how the morphology of specific materials can be related to vibrational shifts. Furthermore, when these spectroscopies and their visual images are combined, it is showed how Raman and FT-IR can complement each other to garner a more comprehensive understanding on complex and multicomponent materials.

Presentation IIC-1

Microstructural Analysis of Welding Slags

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Arc welding is a common industrial method of joining metals together. Many of the arc welding processes utilize fluxes to create a slag that protects the weld metal from the atmosphere and contributes to the weld metal mechanical properties. While welding slags may share similarities with well-known slags used in steelmaking, one particular challenge in understanding welding slags comes from the unusual thermal cycle that they experience during the welding process, with melting and solidification occurring within a few seconds, resulting in extremely non-equilibrium conditions. By analyzing the microstructure of the resulting slag, flux designers can get a better understanding of the phases that form during the welding process, and how these influence the physical and chemical properties of the slag, and consequently, the weld metal. Optical imaging tools, along with SEM + XEDS and XRD methods, have proven to be effective techniques for characterizing the slag. Examples of how these techniques have been used to gain a deeper understanding of welding slags will be illustrated.

Presentation IIIC-2

Detection of Membrane and Cell Wall Targeted Antibiotics Using RedoxSensor Green™

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Identification of bacterial outer membrane targeted antibiotics may identify useful drugs which can be provided in combination with old antibiotics to increase their efficacy, or as scaffolds to build new lethal antibiotics from. We have found that RedoxSensor Green (RSG), marketed as a fluorescent dye for the detection of bacterial reductase activity, may be uniquely suited to identify these compounds. RSG enters the cytoplasm of normal growing *Escherichia coli* without lethality or effecting growth while still reporting upon reductase activity in real time. Upon addition of cell wall and outer membrane (OM) targeting antibiotics, RSG penetration into the cytoplasm increases greatly and produces a consistent high fluorescence signal until failure of the cytoplasmic membrane (CM). This phenomenon occurs for both lethal and non-lethal antibiotics, indicating that the signal is a marker for the disruption of the outer membrane. RSG is both a rapid indicator of the ability of antibiotics to non-lethally disrupt the OM, as well as lethally disrupt the CM. Bactericidal antibiotics show OM disruption coupled with CM failure shortly thereafter while non-bactericidal OM disruption has no associated CM failure. This technique has applications both to screen natural products for OM disruption as well as investigate the efficiency of known bactericidal antibiotics by timing CM failure.

Presentation IIC-3

Low Voltage EDS Using Windowless EXTREME Detector

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Today there is no limitation on the types of materials that can be investigated in the scanning electron microscope; and new improvements in microscope technology, such as low-voltage, have made it common to investigate beam sensitive and non-conductive materials. Also improvements in column and detector design enable low-voltage imaging with excellent spatial resolution and more surface sensitivity. Fortuitously, EDS detector technology, and computer software/hardware, have advanced even faster than the modern SEM. This now allows the acquisition of meaningful analytical data under conditions not previously considered suitable for analysis. A new windowless "EXTREME" detector, designed to increase solid angle collection efficiency, coupled with AZtec software to deconvolute overlapping low energy x-rays, enables EDS analysis at conditions as low as 1kV. Low energy x-rays are enhance, including detection of Li! Also at these low energies, the spatial resolution of EDS falls well below the typical 1-micron teardrop interaction volume, enabling features <10nm to be analyzed. Low energy means the analysis is more surface sensitive, more in tune with the small features observed in SEM imaging. Fast mapping means we study more inhomogeneous materials as well as likely map non-flat and non-dense materials. This requires more critical interpretation of map image data, especially when processed for quantitative results. Automated stage control means we can perform "Large Area Maps", over 1-2 inch areas overnight. This gives us many Gbytes of data that needs user-friendly software to interpret and enable compatible transfer to the non-microscopy community.