FIFTY-SEVENTH ANNUAL MAY CONFERENCE

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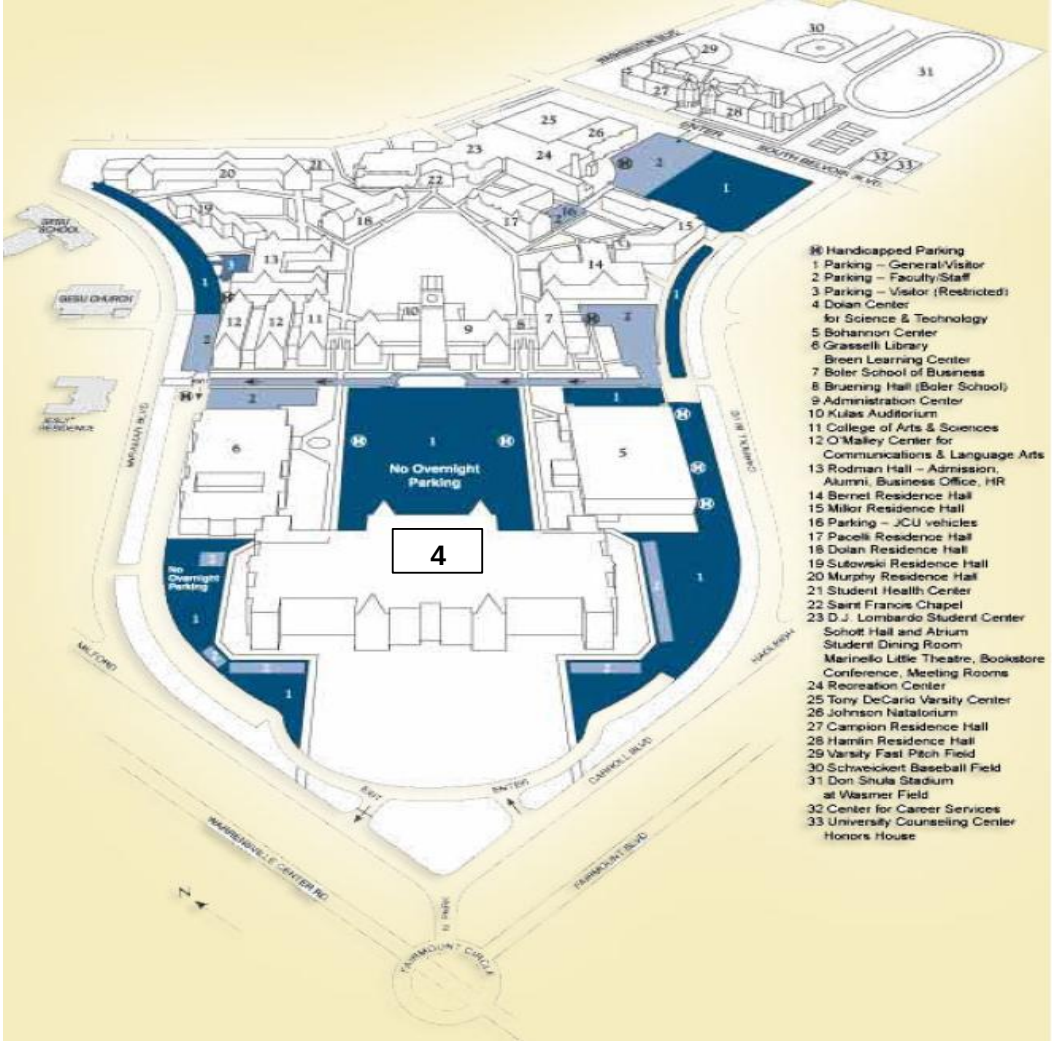
May 15, 2013
Dolan Science Center
John Carroll University
University Heights, Ohio

John Carroll University Campus Map



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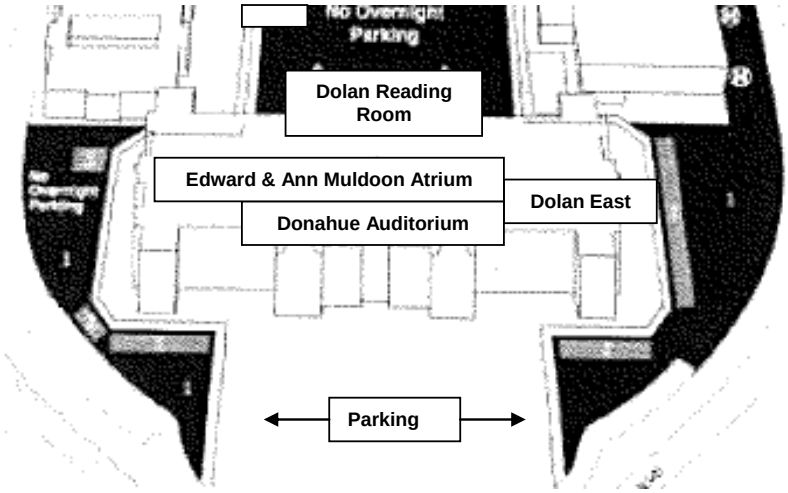

57th Annual
SAS/ACS/MSNO May Conference

May 15, 2013
John Carroll University
Dolan Science Center

PROGRAM

7:00 a.m. **Registration/Continental Breakfast:**
(Edward M. & Ann Muldoon Atrium)

8:00 a.m. **Opening Remarks:** (Donahue Auditorium)
Brian Perry, President, SAS Cleveland Section

Amir Avishai, President, MSNO

Mike Setter, Department Chair, Chemistry, John Carroll University

8:15 a.m. **Invited Address 1:** (Donahue Auditorium)
Chair: Jeanette Killius

Hans Thewissen, *Northeast Ohio Medical University*

"The Walking Whales"

9:15 a.m. **Break (30 minutes):** (Edward M. & Ann Muldoon Atrium)

Presentation Session I

	Session IA **Dolan A202** Chair: Regan Silvestri	**Session IB** **Dolan A203** Chair: Arthur Heuer	**Session IC** **Dolan E130** Chair: Scott Howell
9:45 a.m.	IA-1 "Impact of Cubic ZrW_2O_8 on Polycarbonate Composite" **Xiaodong Gao** *University of Toledo*	IB-1 "Multi-Scale Characterization of How Grain Boundary Structure in Nickel-Based Superalloys Facilitates Deformation" **Jennifer Carter** *Case Western Reserve University*	IC-1 "Incorporating µCT into Studies of Evolutionary Morphology" **Chris Vinyard** *NEOMED*
10:10 a.m.	IA-2 "Synthesis and Characterization of $ZnSnN_2$, a New Semiconductor with a Direct Band Gap of 1.7 eV" **Paul C. Quayle** *Case Western Reserve University*	IB-2 "Revealing Interfaces and Nanostructure: The Application of Atom Probe Tomography to Nickel Based Superalloys" **Chantal Sudbrack** *NASA Glenn Research Center*	IC-2 "3D Imaging of Small Membrane Protein Complexes by Negative Stain Electron Microscopy" **Andreas Engel** *Case Western Reserve University*
10:35 a.m.	IA-3 "Non-hydrolytic Sol-gel Synthesis of Tin Sulfides" **Rajvinder Kaur** *University of Toledo*	IB-3 "Nitrogen-Supersaturated Ferrite in Nitrided 17-7 PH Stainless Steel" **Danqi Wang** *Case Western Reserve University*	IC-3 "Utilizing Imaging Approaches to Interrogate the Cellular Heterogeneity and Communication that Drives the Stem Cell State in Advanced Cancers" **Justin Durla Lathia** *Cleveland Clinic* .

11:00 a.m. **Break (10 minutes):** (Edward M. & Ann Muldoon Atrium)

11:10 a.m. **Yeager Award:** (Donahue Auditorium)
Chair: Rick Kus

Yihui Chen, *Oberlin College*

"Finding Faint Paths in a Dense Jungle: Analysis of the Rotational Structure in Bands in High-Resolution Infrared Spectra to Determine Accurate Structures"

11:40 p.m. **Lunch:** (O'Connell Reading Room)

12:45-1:45 p.m. Poster Session: (Second Floor Hallway)

Presentation Session II

	Session IIA **Dolan A202** Chair: Rick Kus	**Session IIB** **Dolan A203** Chair: Jonathan Cowan	**Session IIC** **Dolan E130** Chair: Grahame Kidd
1:50 p.m.	IIA-1 "Quantitative Analysis of Additives in Polymers by Thermal Desorption and Reactive Pyrolysis" **Dave Randle** *Frontier Labs*	IIB-1 "Advancements in Imaging Technology and Characterization for Transmission Electron Microscopy" **Stephen Mick** *Gatan*	IIC-1 "CryoEM and MDFF Modeling of the Circadian Clock KaiBC Complex from S. Elongatus" **Seth Villarreal** *Case Western Reserve University*
2:15 p.m.	IIA-2 "Characterization of Stereo-Sequences in Poly (Vinyl Fluoride) by $^{1}H/^{13}C/^{19}F$ 3D-NMR" **Linlin Yi** *University of Akron*	IIB-2 "Silane Modification of Oxides for Biological and Energy Applications" **Ina Martin** *Case Western Reserve University*	IIC-2 "Mobility and Clustering in Biological Membranes Using Time Resolved Fluorescence Microscopy" **Adam W. Smith** *University of Akron*
2:40 p.m.	IIA-3 "Characterization of GTDI Soot and Comparison with Diesel Soot" **Monica Ford** *The Lubrizol Corporation*	IIB-3 "Direct Observation of Smectic Layers in Thermotropic Liquid Crystals" **Cuiyu Zhang** *Kent State University*	IIC-3 "Chromosome Dynamics During Meiosis – Integrating Structure and Function" **Valentin Boerner** *Cleveland State University*
3:05 p.m.	IIA-4 "Tribological Studies on KG-80 as a Space Lubricant" **Ken Street** *NASA-Glenn Research Center*	IIB-4 "Resistance and Seebeck Coefficient Measurements on Single Crystal $ZnGeN_2$ Rods" **Jeff Dyck** *John Carroll University*	IIC-4 "Spider Adhesion" **Ali Dhinojwala** *University of Akron*

3:30 p.m. **Break (20 minutes):** (Edward M. & Ann Muldoon Atrium)

Presentation Session III

	Session IIIA **Dolan A202** Chair: Marcus Tirado	**Session IIIB** **Dolan A203** Chair: Sunniva Collins	**Session IIIC** **Dolan E130** Chair: David Hovis
3:50 p.m.	IIIA-1 "Analysis of Gold Nanoparticles Using the NexION 300 ICP-MS in Single Particle Mode" **Lorraine Foglio** *Perkin Elmer*	IIIB-1 "Nanostructural Evolution of Hard Turning Layer in Carburized Steels" **Vikram Bedekar** *Timken*	IIIC-1 "Integrating Inelastic Light Scattering Modalities for Biomaterials Research" **Jonathan R Damsel** *Cleveland State University*
4:15 p.m.	IIIA-2 "Ten Years of Advances in X-ray Energy Dispersive Spectroscopy" **John Konopka** *ThermoFisher Scientific*	IIIB-2 "Materials and Processes in the Manufacture of Civil War Small Arms" **John C. Harkness** *Retired/Materion*	IIIC-2 "A New Multi-Technique Workstation Featuring A Plasma Ion Source" **Ed Principe** *Tescan*
4:40 p.m.	IIIA-3 "Auger Electron Spectroscopy Characterization of Interstitially Hardened Stainless Steels" **Wayne Jennings** *Case Western Reserve University*	IIIB-3 "Low-Temperature Acetylene-Based Carburization of 316L Austenitic Stainless Steel" **Yindong Ge** *Case Western Reserve University*	IIIC-3 "Correlating Gas Concentration Polarization with Microstructures of Porous SOFC Cathodes using Avizo XLab Hydro" **Christian Wietholt** *FEI – Iviso*

5:05 p.m. **Break (15 minutes):** (Edward M. & Ann Muldoon Atrium)

5:20 p.m. **Best Student Paper/Poster Awards**
Amir Avishai

5:30 p.m. **Morley Lecture** (Donahue Auditorium)
Chair: Mark Waner

Peter Wipf, University of Pittsburgh

"A Tale of Two Drug Candidates"

6:30 p.m. **Reception** (Edward M. & Ann Muldoon Atrium)

7:10 p.m. **Program** (O'Connell Reading Room)

Recognition of Meeting Sponsors – Bob Williams

Bell Award Presentations – Tom Steele

Morley Award Presentation – Mark Waner

Closing Comments – Brian Perry

7:30 p.m. **Dinner** (O'Connell Reading Room)

2013 May Conference Planning Committee

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Student Paper Awards	Melanie Knowlton, LORD Corporation Kevin Otteni, LORD Corporation Min Gao, Kent State University Jeanette Killius, NEOMED
Student Posters	Chris Holp, FirstEnergy Wayne Jennings, Case Western Reserve University Marcus Tirado, LORD Corporation George Marton, LORD Corporation Tom Steele, Lubrizol Corporation
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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	1988	Joy Gorecki
1963	John H. Konnert	1989	Sheryl Tucker
1964	Sheldon J. Green	1990	No Award Given
1965	Cheryl H. Miller	1991	Stephen C. Stone
1966	Dale Wingeleth	1992	No Award Given
1967	Richard D. Ash, Jr.	1993	Baonian Hu
1968	Jon Mynderse	1994	Amy L. Lusk
1969	Virginia E. Coates	1995	John W. Cave
1970	Charles F. Cobb	1996	Michael Fiorentino
1971	Gerald R. Cappo	1997	Jonathan Flad
1972	Donald R. Diehl	1998	Christopher S. Callam
1973	Fred A. Fortunato	1999	David T. Clark
1974	Douglas B. Rahrig	2000	Adam Van Wynsberghe
1975	William Hart	2001	David C. Oertel
1976	John Havens	2002	Richard L. Barger, Jr.
1977	Thomas M. Leiden	2003	Michelle Adams
1978	Scott A. Raybuck	2004	Tiffany Leigh Copeland
1979	Jeff Weidenhamer	2005	Stacey Lynne Dean
1980	Alexander Kondow	2006	Colleen M. Burkett
1981	Raymond E. Cline	2007	Manasi Bhate
1982	Marie Zaper	2008	Nikolas Joseph Neric
1983	Brian L. Cousins	2009	Deacon J. Nemchick
1984	Ka-Pi Hoh	2010	Rachel V. Bennett
1985	Chris Scott	2011	Daphne A. Guinn and Jennifer L. Miller
1986	Ann M. Mulichak	2012	Jean Quenneville
1987	Rex Ramsier	2013	Yihui Chen

2013 Ernest B. Yeager Award Recipient

Yihui Chen
of
Oberlin College

"Finding Faint Paths in a Dense Jungle: Analysis of the Rotational Structure in Bands in High-Resolution Infrared Spectra to Determine Accurate Structures"

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 Horejis	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

The 2013 John Bell Memorial Award Recipient

Grace Gamble

Can a Vegetable's Method of Preservation be Defined by its Ratio of Chlorophyll A to Chlorophyll B?

The 2013 John Bell Memorial Merit Award Recipient

Justin Boes

Does Glucose, a Chiral Molecule, Affect the Plane of Polarized Light?

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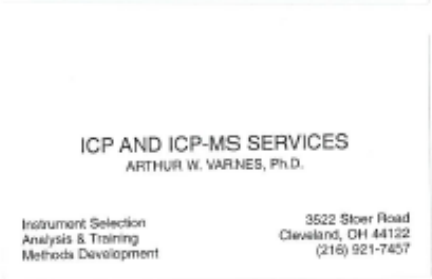

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Joint Session I

THE WALKING WHALES

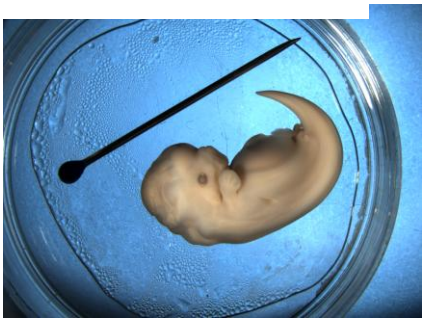
HANS THEWISSEN, PH.D.
Ingalls-Brown Professor of Anatomy
Northeast Ohio Medical University

thewisse@neomed.edu

Dr. Thewissen's research concerns modern and fossil whales, and he is a specialist on the first 13 million years of whale evolution, a period when the ancestors of whales, which looked like tiny deer, became aquatic. He will introduce a variety of early whales, some resembling otters, others alligators or seals, and include the transitions that led to the origin of whales looking like modern forms.

Dr. Thewissen's uses micro CT technology to unravel the finer anatomy of fossil and recent whales. His current research attempts to determine the shape of the inner ear of bowhead and beluga whales in Alaska. Tools such as the micro CT provide a powerful way to study evolution.

About the speaker:
A native of the Netherlands, Dr. Thewissen holds graduate degrees in biology and geology and teaches anatomy and embryology to medical students. He has funded research projects in paleontology and anatomy. His research covers the evolution of mammals, particularly whales. Since 1985, Dr. Thewissen has conducted fossil digs in India and Pakistan, where he has unearthed the fossils of the earliest relatives of today's whales. He also goes to Alaska to study modern whales and their adaptations to the changing arctic climate.



Dr. Thewissen has been credited with discovering the "missing link" in whale evolution by S. J. Gould. His work has had a profound impact on how scientists understand the process of evolution and is referred to in many college textbooks.

Presentation IA-1

Impact of Cubic ZrW_2O_8 on Polycarbonate Composite

Xiaodong Gao and Cora Lind-Kovacs
Department of Chemistry
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Cubic ZrW_2O_8 is a material that exhibits isotropic negative thermal expansion (NTE). It has been used to control the thermal expansion of polymers. The reduction of the polymer thermal expansion can be attributed to two factors: (a) the thermal motion of the polymer chains is constrained by the particles mixed with the polymer; (b) the NTE of the particles also lowers the composite expansion. However, the exact contribution from each factor is unknown, and thus will be studied in this project. This goal is achieved by a direct comparison of two composites, one of which utilizes ZrW_2O_8 as filler particles, and one of which uses $ZrW_2O_7(OH)_2{\cdot}2H_2O$ particles with identical morphology as ZrW_2O_8, but with positive thermal expansion. Therefore, the effect of chain constraints can be eliminated, and the NTE effect can be found. Polycarbonate was chosen as a polymer matrix in this work. ZrW_2O_8 was obtained by converting a precursor, $ZrW_2O_7(OH)_2{\cdot}2H_2O$, via a topotactic transformation. The precursor was synthesized via a hydrothermal method, enabling particle size control. The thermal expansion coefficient of the precursor was determined using variable temperature x-ray diffraction combined with Rietveld refinement. To improve the interaction between the particles and matrix, the filler particles were modified by grafting polycarbonate oligomers onto the surface via an *in-situ* polymerization. Excess triphosgene monomer has to be used to make the polymerization happen on the surface, which is less favorable than the very similar reaction with the second monomer in solution. Interestingly, for the modification of the precursor, the surface reaction only succeeded on particle with small crystallite size. The surface of fully crystallized particles could not react with the monomers. The modified particles were then mixed with commercial polycarbonate by a reprecipitation blending method, followed by casting a free standing film from dichloromethane. However, additional care was required to prevent polycarbonate from crystallizing during solution based casting. An in-house designed vessel was used to reduce the air content, and to accelerate the evaporation of dichloromethane. The homogeneity of the composite films was tested by thermogravimetric analysis. The films were cut by microtome, and examined by scanning electron microscopy. The linear thermal expansion coefficient of two different films will be determined using dynamic mechanical analysis.

Presentation IA-2

Synthesis and Characterization $ZnSnN_2$, a New Semiconductor with a Direct Band Gap of 1.7 eV

Paul Quayle and Kathleen Kash
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Case Western Reserve University
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Cleveland, OH 44106

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There has been much research and development devoted to the $In_xGa_{1-x}N$ system of alloy semiconductors for photovoltaic applications in the last decade, as well as for photocatalytic applications[1], given the potential of the system to harvest solar energy throughout the 0.7-3.4 eV range. In addition, there are many ongoing efforts to improve the efficiency of longer wavelength nitride light emitting diodes. However, there are still challenges in realizing these applications, including, but not limited to, phase separation in the intermediate alloy range and difficulties in scalability due to the rising cost and restrictions on the availability of indium. Here we report the synthesis of a new direct band gap semiconductor, $ZnSnN_2$, that, as the low-band-gap member of the $Zn(Si,Ge,Sn)N_2$ alloy family of semiconductors, enables us to now consider addressing some of these challenges with an alternative earth-abundant materials system with direct band gaps that span the energy range from 1.7 to 4.5 eV.[2] We describe our plasma-assisted vapor-liquid solid growth technique, used to produce polycrystalline material with average crystallite sizes of 70 nm. We describe the growth conditions that produce $ZnSnN_2$ while avoiding production of the competing zinc and tin nitrides, and the spectroscopic and Auger chemical analysis methods used to distinguish the three competing phases. We report on the structure and lattice parameters of $ZnSnN_2$, as determined by x-ray diffraction spectroscopy, and the band gap, measured by photoluminescence excitation spectroscopy to be 1.7 ±0.1 eV.

[1] T. Nakano, M. Hamada, S. Fuke, Fabrication and performance of photocatalytic GaN powders, *Advanced Materials Research* **222**, 142 (2011).
[2] A. Punya, W.R.L. Lambrecht, M. van Schilfgaarde, Quasiparticle band structure of Zn-IV-N2 compounds, *Phys. Rev. B* **84**, 165202, 2011.

Presentation IA-3

Non-hydrolytic Sol-gel Synthesis of Tin Sulfides

Rajvinder Kaur and Cora Lind-Kovacs
Department of Chemistry
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Non-hydrolytic sol-gel synthesis of tin sulfides: The tin sulfide system shows three binary phases, SnS, SnS_2 and Sn_2S_3, in the phase diagram. Tin sulfides belong to the class of IV-VI semiconductors, and adopt layered structures. They are considered promising candidates for photovoltaic applications, as they are environmentally benign, inexpensive and abundant. Due to their potential applications as electrode materials for Li ion batteries, lubricants, photoconductors, photocatalysts, and absorber layer materials in photovoltaic solar cell devices, tin sulfides are gaining importance as a research area. All these applications strongly depend on various features like homogeneity, controlled oxidation states, high surface area and purity of the materials. To achieve some of these, a low temperature synthetic route is required. A variety of low temperature methods are being explored due to the increased demand for advanced materials. This project focuses on exploring non-hydrolytic sol-gel synthesis of tin sulfides. It is a solution based method that can be used for the synthesis of crystalline tin sulfides under oxygen free conditions. All reaction parameters can be fine tuned to obtain particular polymorphs of the system, and all three thermodynamically stable phases have been obtained. In addition, low temperature approaches can result in formation of metastable, previously unknown polymorphs. Current results indicate that such phases may exist in the tin sulfide system as well.

Presentation 1B-1

Multi-scale Characterization of How Grain Boundary Structure in Nickel-based Superalloys Facilitates Deformation

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As the potential operating temperature of polycrystalline nickel-based superalloys increases, the grain boundary structure plays a more dominant role in the deformation mechanisms of these materials. In this work, the effect of grain boundary character (special boundaries, grain boundary serration) on the strain accumulation behavior in these materials was tested under constant loading conditions. The nature of grain boundaries necessitates the need of multi-scale experimental techniques to characterize the deformation properties of both the network and individual boundaries. We couple full field strain mapping with site-specific 3D microstructure and transmission electron microscopy analysis to characterize deformation at boundaries with different character. We confirm that an engineered grain boundary structure can dramatically transform how a nickel-based superalloy deforms, with particular emphasis on structural affects on grain boundary sliding phenomena.

Presentation IB-2

Revealing Interfaces and Nanostructure: The Application of Atom Probe Tomography to Nickel-based Superalloys

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Precipitation strengthened nickel-based superalloys are used to fabricate turbine-components for aeronautical jet engines, commercial and military, and land-based gas-turbines engines because of their excellent mechanical properties at elevated temperatures. The ability to control microstructure stability of these complex alloy systems requires an understanding of the fundamental aspects of precipitate evolution. With the ability to locate and identify atoms in three dimensions, atom-probe tomography (APT) is providing unparalleled insights into interfaces and nanostructure. This presentation will focus on the application of APT to both model and commercial nickel-base superalloys. For complex commercial alloys, determining the diffusional pathways is not a trivial task, but by selecting model systems the problem becomes tractable, both experimentally and with sophisticated atomistic modeling. The Ni-Al-Cr system is particularly attractive because it is the ternary system that fundamentally underpins commercial superalloys, where the thermodynamic and kinetic parameters have been well characterized. The high temperature strength in these alloys is a direct consequence of the elastically hard γ' -precipitates of $Ni_3(Al_xCr_{1-x})$ in an fcc chromium-rich γ solid solution.

Presentation IB-3

Nitrogen-supersaturated Ferrite in Nitrided 17-7 PH Stainless Steel

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Low-temperature nitridation has been successfully applied on 17-7 precipitate-hardening stainless steel. After moderate or high nitrogen activity (≥ 7400) nitridation, delta ferrite grains within the interstitially hardened case show uniform in contrast, so-called "featureless grains". Chemical analysis shows these featureless ferrite grains possess significant amounts of nitrogen. Diffraction patterns taken from the featureless grains show that the ferrite grains still possess BCC lattice characteristic and another set of spots indicates the formation of second phase. The coherent phase is identified as MN with the rocksalt structure, obeying Bain's orientation relationship. However, after low nitrogen activity (~3000) nitridation, needles were observed in the ferrite grain with the "featureless" matrix. The second phase with the needle-like morphology has been identified as M_2N.

Presentation IC-1

Incorporating µCT Into Studies of Evolutionary Morphology

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Affordable µCT has revolutionized how biologists study morphology as this technology allows detailed, non-invasive assessment of form. Here we consider two project incorporating µCT in evolutionary morphology research. The first project examines the genetic architecture of skeletal form by documenting the quantitative genetics of mouse mandibular cross-sections and searching for QTL (Quantitative Trait Loci) underlying mandibular form across inbred strains of mice. The second study looks at load-resisting performance in the mandibles of primates incorporating µCT to provide detailed links between symphyseal morphology and strength. Both studies illustrate how µCT can be effectively integrated in 21st century anatomical studies.

Presentation IC-2

3D Imaging of Small Membrane Protein Complexes by Negative Stain Electron Microscopy

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Aquaporins are ubiquitous membrane proteins involved in the water homeostasis of all organisms. These proteins have a mass of around 30 kDa, form tetramers, and many have been crystallized either in 2D or 3D arrays. We were interested to visualize solubilized tetramers in 3D to determine the size and shape of belts formed by different detergents. 3D EM of negatively stained samples proved to provide this information.

Rhodopsin (Rho) is densely packed in disc membranes that are stacked like micron-sized pancakes in the rod outer segments of retinal photoreceptors. A single photon activates Rho to Rho*, which binds the heterotrimeric transducin (G_t) inducing G_t activation and dissociation. Down-stream events amplify the photon-induced signal to ultimately produce a detectable electric pulse.

Solubilization of native Rho dimers and *in-vitro* reconstitution of the Rho*-G_t complex in the nucleotide-free arrested state made it possible to isolate and characterize the active Rho*-G_t complex, whose mass determined by scanning transmission electron microscopy is 221±12 kDa. The 21 Å molecular envelope calculated from projections of negatively stained Rho*-G_t complexes accommodates two Rho molecules and one G_t heterotrimer, demonstrating the heteropentameric structure of the Rho*-G_t complex.

Presentation IC-3

Utilizing Imaging Approaches to Interrogate the Cellular Heterogeneity and Communication that Drives the Stem Cell State in Advanced Cancers

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Advanced cancers display a high degree of cellular heterogeneity and are organized in a hierarchy that resembles a normal organ. At the apex of this hierarchy is a self-renewing, therapeutically resistant, tumorigenic cancer stem cell (CSC). CSCs have been characterized in many advanced cancers including glioblastoma multiforme (GBM), the most prevalent and malignant primary brain tumor for which no current cure exists. Integrating the concept that advanced cancers contain a CSC population has provided additional insight into the dynamics of tumorigenic processes and identified novel therapeutic targets. A critical barrier to this integration has been interrogating CSCs in the context of their microenvironment, which itself provides essential maintenance signals. To overcome this barrier, we have developed several imaging approaches that have been informative at single cell resolution. Using these approaches, we provided the first functional evidence of elevated in vivo tumor formation of CSC derived from GBM using multiphoton imaging. We have built upon this work to evaluate the effect of therapies on CSCs. We have also adapted many of these imaging approaches to study cell-cell communication, a key regulator of cellular phenotypes. Our data suggest that a vast network exists within a tumor and that cell-cell communication is vital of CSC maintenance and therapeutic resistance. The CSC hypothesis adds an additional layer of complexity to cancer and by integrating imaging approaches into our studies, our objective is to interrogate how CSCs contribute to tumor maintenance with the objective of identifying novel targets for GBM and other advanced cancers.

Yeager Award Presentation

Finding Faint Paths in a Dense Jungle: Analysis of the Rotational Structure in Bands in High-Resolution Infrared Spectra to Determine Accurate Structures

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Detecting subtle electronic effects on the structures of molecules depends on determining structures accurate to 0.001 Å. Most structure determinations, such as by diffraction methods, are blurred at approximately 0.02 Å. Accurate structures may be determined as semi-experimental structures, which depend approximately 99% on rotational constants obtained from high-resolution rotational spectroscopy and 1% on spectroscopic alphas obtained from high-level quantum chemical calculations. For non-polar molecules, rotational constants must be obtained from rotational structure in infrared spectra. The use of a Loomis-Wood pattern recognition program is integral in assigning quantum numbers in the dense vibration-rotation spectra. Assigned lines are then fit to a Watson-type rotational Hamiltonian to yield rotational constants. Isotopic substitution is necessary to obtain a full set of rotational constants to provide enough information for all the molecular parameters. A structure is finally fit to the set of rotational constants. This method is being applied to the 1,3,5-hexatriene system to investigate the effects of π-electron delocalization in polyenes.

Presentation IIA-1

Quantitative Analysis of Additives in Polymers by Thermal Desorption and Reactive Pyrolysis

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Quantitative analysis of additives in polymers using a temperature programmable micro-furnace based pyrolyzer (Frontier Lab EGA/PY-3030D) and detection by GC/MS will be discussed. Examples will be shown using thermal desorption (TD) and reactive pyrolysis (RxPy) for Irganox 1076 and 1010 in polyethylene. A new ASTM Method D-7823: Standard Test Method for the Determination of Low Level, Regulated Phthalates in Poly (Vinyl Chloride) Plastics by Thermal Desorption - GC/MS, will also be discussed.

Presentation IIA-2

Characterization of Stereo-Sequences in Poly (Vinyl Fluoride) by $^{1}H/^{13}C/^{19}F$ 3D-NMR

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Tacticity has an enormous influence on the physical and chemical properties of polymers. There is considerable work using 1D-NMR and empirical rules to study the stereo-sequences in polymers. This work suggests that $^{1}H/^{13}C/^{19}F$ 3D-NMR experiments can provide superior resolution and atomic connectivity information, so that unambiguous resonance assignment can be made for poly(vinyl fluoride) (PVF). Compared to prior work on 3D-NMR studies of stereosequence effects in fluoropolymers, the 3D-NMR pulse sequence used in this work is based on single quantum coherence transfer, which eliminates the complicated splitting patterns resulting from evolution of multi-quantum coherence. In addition, selective excitation of the ^{19}F nuclei of interest significantly reduces the folding of peaks from other spectral regions. This greatly simplifies the spectra and makes the assignment of resonances much easier. Based on our results, it is possible to assign the ^{19}F resonance to the pentad level.

Presentation IIA-3

Characterization of GTDI Soot and Comparison with Diesel Soot

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In the quest to improve fuel economy in gasoline engines, automotive manufacturers are producing more gasoline turbocharged direct injection engines (GTDI). One unintended byproduct of this operation is the increased generation of soot compared to PFI in the engines, which can lead to increased wear in engine components similar to that observed in diesel engines.

In this work, we compare physical and chemical characteristics of GTDI soot with diesel soot. Drains from several vehicles equipped with GTDI, diesel engines and dyno tests are collected in order to characterize soot in oil. Exhaust soot is also collected and characterized. X-ray fluorescence, X-ray photoelectron spectroscopy, high resolution transmission electron spectroscopy, and Raman spectroscopy are among the techniques used for characterization.

Presentation IIA-4

Tribological Studies on KG-80 as a Space Lubricant

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In the earlier days of space tribology, conventional mineral oils were employed but failed quickly, promoting the search for lubricants with better friction coefficients, vapor pressures and lifetimes, among other properties. Although a number of superior liquid lubricants are currently available, e.g. Pennzanes and perfluoropolyalkylethers, some of the older mineral oil derived lubricants, such as KG-80, are still used in niche space applications. KG-80 is a super refined mineral oil which was developed in the 1960's and has not been manufactured since the 1970's. In spite of these drawbacks, there are still supplies of KG-80 persisting and it is still used in the International Space Station Control Moment Gyroscopes. In this paper we report on Spiral Orbit Tribometry studies of the lifetime and friction coefficient for this oil on bearing steel. We also report on the molecular weight and distribution and the vapor pressure at relevant space application temperatures.

Presentation IIB-1

Advancements in Imaging Technology and Characterization for Transmission Electron Microscopy

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TEM imaging options continue to evolve rapidly. Pixel count and frame rates are increasing and higher data collection efficiency is being realized. As imaging performance improves, it becomes increasingly important to understand the inherent advantages and limitations of each available technology. This talk will give an overview of the fundamental TEM camera technologies that are available today and provide guidelines to help identify the best camera for a given application.

Presentation IIB-2

Silane Modification of Oxides for Biological and Energy Applications

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Silane molecules have tremendous utility for bridging inorganic and organic materials in applications ranging from DNA microarrays to photovoltaics. Control of the composition, chemistry and structure of the silane film is crucial for optimization of the final devices. X-ray photoelectron spectroscopy (XPS) and spectroscopic ellipsometry (SE) were used to characterize the chemical composition and thickness of thin silane films, including 3-aminopropyldimethylethoxysilane (APDMES), 3-aminopropyltriethoxysilane (APTES), and allyl-triethoxysilane (ATES). APDMES and APTES were used for DNA attachment to silica, and the silane film structure was shown to play a role in the DNA hybridization efficiency. APTES, APDMES and ATES were used to modify transparent conductive oxides (TCO) for photovoltaic applications. Varying the silane reaction conditions allowed for control of film thickness and functional groups, resulting in varying surface energies, without significant changes to the transparency of the TCO. The effects of damp heat and hot irradiance on ATES functionalized TCOs will be reported.

Presentation IIB-3

Direct Observation of Smectic Layers in Thermotropic Liquid Crystals

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Cryo - Transmission Electron Microscopy (cryo-TEM) is a well developed technique to study biological materials and lyotropic liquid crystals with resolution down to about 2-3 nm.[1] Nanostructures of thermotropic liquid crystals are usually studied by freeze-fracture TEM (FFTEM), where the surface of a fractured cryo-fixed sample is coated by layers and the resulting replica film is imaged. This method can provide a resolution of about 2 nm. To study details of smectic layers of bulk thermotropic liquid crystals, the TEM resolution has to be better than 1 nm. Here we demonstrate cryo-TEM imaging of smectic liquid crystal layer spacing with resolution better than 0.7nm. Our results show perfect periodicity over several hundred layers in the smectic phase, and also show the first direct evidence of smectic clusters on length scales of 30-50 nm in a nematic liquid crystal. The results are in complete agreement with SAXS measurements. The observation of smectic clusters in the nematic phase is of special interest in bent-core liquid crystals [2], where the smectic clusters are stable over wide temperature ranges [3], in contrast to the well-known pretransitional “cybotactic” clusters [4] that appear only in the vicinity of a bulk smectic phase.

We also study the nanofilaments (B4 phase) and the modulated smectic layers (B7 phase) of various bent shaped liquid crystal compounds by using cryo-TEM. In the B4 phase a periodic array of about 8~10 nm wide bands of parallel stripes, separated by a distance equal to the layer spacing, appear with a periodicity of about 120 nm corresponding to the half pitch of the nanofilaments. As cryo-TEM shows only layers that are parallel to the electron beam, these results indicate grains of straight layers twisted along the filament axis compose the nano-filaments. In the B7 phase cryo-TEM not only can visualize the smectic layers, but also the periodic modulation indicating defects with less dense molecular packing. In addition we observe a labyrinth structure with curvature radii in the 150 nm ranges. These results yield information complementary to freeze fracture TEM and X-ray observations.

Presentation IIB-4

Resistance and Seebeck Coefficient Measurements on Single Crystal $ZnGeN_2$ Rods

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$ZnGeN_2$ is a II-IV-nitride analog to the III-nitride semiconductor GaN, and the two share very similar crystal structures, lattice parameters, and band-gap energies. Along with these commonalities, $ZnGeN_2$ has a number of distinctly different predicted properties, in particular its doping and defect properties, nonlinear optical properties, and lower spontaneous polarization coefficients. Recently, bulk single crystals of $ZnGeN_2$ have been synthesized via a vapor-liquid-solid method, but transport measurements have not been reported. In this work, we present electrical resistance and Seebeck coefficient (S) data on 3-micron diameter single crystal rods of $ZnGeN_2$. A custom designed stage enabling two-probe transport measurements under the influence of a temperature gradient was developed, and sample preparation was aided by a focused ion beam technique for forming electrical contacts. Two-probe resistance data show that the Pt contacts to the crystals are Ohmic. Measurements of Seebeck coefficient imply that the dominant charge carriers are electrons, and the carrier gas is degenerate. The data will be compared to available band structure calculations and the potential for use of this compound as a thermoelectric material will be discussed.

This work is supported by NSF grant DMR-1006132.

Presentation IIC-1

CryoEM and MDFF Modeling of the Circadian Clock KaiBC Complex from *S. Elongatus*

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The metabolisms of most living things are regulated by circadian rhythms, cycles of activity and biological processes with periods of 24 hours. These biological clocks exist in varying degrees of complexity. Humans have a complex biochemical clock, involving numerous components. In comparison, the cyanobacteria, Synechococcus Elongatus, uses a clock composed of only three proteins. Understanding the protein-protein interactions and conformational changes of even this simple molecular clock has proven difficult. While crystal structures exist for these three proteins, the complexes formed during the cycling of KaiC phosphorylation status are not characterized at high resolution. Molecular modeling techniques, guided by experimentally determined cryoEM density maps, provide an avenue to predict and examine the interacting surfaces of these three proteins. This offers the opportunity for greater insight into the molecular mechanisms required for a 24 hour circadian rhythm.

Using a moderate resolution cryoEM density map of the KaiBC complex to flexibly fit separate crystal structures together within a single simulation, we predict the protein-protein interacting surfaces and important residues of the KaiBC complex. Several residues of KaiC and KaiB are suggested as key to the role of KaiB binding and influencing the KaiC phosphorylation state.

Presentation IIC-2

Mobility and Clustering in Biological Membranes Using Time Resolved Fluorescence Microscopy

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Fluorescence microscopy is a powerful tool for live cell imaging, but it remains challenging to quantify the structure and dynamics of membrane receptor complexes. This is because the protein clusters undergo complex translational dynamics and are smaller than the optical diffraction limit. Recent breakthroughs in sub-diffraction limit fluorescence imaging make it possible to study membrane protein complexes with higher resolution, but it is still difficult to measure correlated, dynamic assembly. I will present work using two-color fluorescence microscopy with time-correlated single photon counting (TCSPC) to measure the oligomerization state of epidermal growth factor receptors (EGFR) in live cells. Using a pulsed interleaved excitation scheme, it is possible to quantify the monomer-dimer population of EGFR in live cells with high accuracy. The results demonstrate that EGFR is primarily monomeric in the plasma membrane, with only a small percentage of cells showing an appreciable dimer population. This approach represents a powerful experimental platform to measure protein-protein and protein-lipid interactions in live cells.

Presentation IIC-3

Chromosome Dynamics During Meiosis – Integrating Structure and Function

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In the germ line of all sexually reproducing organisms, the genome size is reduced by half via a specialized cell division called meiosis. Reductional segregation of homologous chromosomes during the first meiotic division generates haploid gametes from diploid precursor cells. Meiotic genome reduction ensures that upon gamete fusion, the genome size stays constant rather than doubling. The Börner lab combines genetic approaches, physical analysis of chromosomal DNA and immunofluorescence microscopy to understand function and mechanism of changes in chromosome structure during meiosis. Two universally conserved, intimately related cellular processes are critical for meiotic chromosome segregation: First, crossovers form between homologous chromosomes mediating their attachment to opposite spindle poles in addition to their role in generating novel allelic combinations. Second, the synaptonemal complex assembles between homologous chromosomes, connecting chromosomes via a protein scaffold while crossover formation is ongoing. Defects in crossover formation and synaptonemal complex assembly are associated with aneuploid gametes, resulting in infertility, still birth and birth defects. I will discuss (i) roles of the synaptonemal complex at various steps of crossover formation and (ii) mechanisms that control assembly and functionality of the synaptonemal complex.

Presentation IIC-4

Spider Adhesion

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Spiders employ clever behavioural strategies combined with almost invisible custom-made adhesive silk fibers to spin webs for capturing preys and for locomotion. The adhesives used in these webs have evolved over millions of years into a class of natural materials with outstanding properties. In my presentation, I will review how spiders use different adhesives to capture prey and locomotion. The spiders take advantage of the mechanical properties of the silk threads, the physical structure, the presence of salts, and the chemistry of the glue to enhance adhesive forces. Understanding how spiders have evolved to design materials provides important insights in designing new synthetic adhesives.

Presentation IIIA-1

Analysis of Gold Nanoparticles Using NexION 300 ICP-MS in Single Particle Mode

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Engineered Nanomaterials (ENMs) are synthesized by a manufacturing process that produces and controls ENMs to have at least one dimension in the range of 1 to 100nm in size. ENMs often possess different properties than bulk materials of the same composition, making them of great interest to a broad spectrum of industrial and commercial applications. The widespread use and application of ENMs will inevitably lead to their release into the environment, which raises concern about their potential adverse effects on the ecosystems and, subsequently, human health. To better understand ENMs in the environment, the following ENM characteristics will aid in this assessment: concentration, composition, particle size, shape, and other surface characteristics.

This work describes the theory and application of Single Particle- ICP-MS in analyzing Metal Based Nanoparticles. Single Particle (SP-ICP-MS) allow the differentiation between ionic and particulate signals, quantitate both the ionic and particulate fraction, measures particle concentration (part/mL), particle sizes (if shape is known), and explores agglomeration and size distribution.

SP-ICP-MS is a key analytical instrument in assessing the fate, behavior and distribution of (ENMs) in several types of matrices (environment, food, etc.), evaluating ENMs bioavailability and bioaccumulation in the biota, and improving bio-labeling capabilities and advancements in the medical field.

Presentation IIIA-2

Ten Years of Advances in X-ray Energy Dispersive Spectroscopy

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In the past decade EDS has seen revolutionary changes in detectors, electronics and software. Computer and storage improvements have radically altered the way data is collected, stored and processed. This has resulted in major improvements in throughput and sensitivity strengthening traditional capabilities such as light element quantitative analysis while new algorithm have added capabilities such as post processing of x-ray maps and automatic parsing of phases. This talk will detail those changes and illustrate them with examples.

Presentation IIIA-3

Auger Electron Spectroscopy Characterization of Interstitially Hardened Stainless Steels

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Interstitially hardened stainless steels are important materials for many reasons. In particular, stainless steels that have been carburized by low temperature interstitial hardening have superior mechanical properties of increased hardness and toughness while retaining and even improving corrosion resistance. Characterization of these materials by Auger Electron Spectroscopy is complicated by carbon contamination, continuous sputtering and subsequent differential sputtering effects. Resolution of this by the use of modified Relative Sensitivity Factors is necessary for accurate Auger line scans. This work details the procedures for these corrections for type 316 stainless steels and other carburized materials.

Presentation IIIB-1

Nanostructural Evolution of Hard Turning Layer in Carburized Steels

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The mechanisms of failure for components subjected to contact fatigue are sensitive to the structure and properties of the material surface. Although, the bulk material properties determined by the steel making, forming and the heat treatment; the near surface material properties are altered during final material removal processes such as hard turning or grinding. Therefore, the ability to optimize, modulate and predict the near surface properties during final metal removal operations would be extremely useful in the enhancement of service life of a component.

Hard machining is known to induce severely deformed layers causing dramatic microstructural transformations. These transformations occur via grain refinement or thermal transformation depending upon cutting conditions. The aim of this work is to engineer the near surface nanoscale structure and properties during hard turning by altering strain, strain rate, temperature and incoming microstructure.

The near surface material transformations due to hard turning were studied on carburized SAE 8620 bearing steel. Variations in parent material microstructures were introduced by altering the retained austenite content. The strain, strain rate and temperature achieved during final metal cutting were altered by varying insert geometry, insert wear and cutting speed. The subsurface evolution was quantified by a series of advanced characterization techniques such as transmission electron microscopy (TEM), glancing angle X-ray diffraction GAXRD), X-ray stress and nanoindentation which were coupled with numerical modeling.

Results showed that the grain size of the nanocrystalline near surface microstructure can be effectively controlled by altering the insert geometry, insert wear, cutting speed and the incoming microstructure. It was also evident that the near surface retained austenite decreased at lower cutting speed indicating transformation due to plastic deformation, while an increase in the retained austenite at higher cutting speed indicated thermal transformation. Nanoindentation tests showed that the substructures produced by plastic deformation follow the Hall-Petch relationship while the structures produced by thermal transformation did not. This indicated a change in the hardness driver from dislocation hardening to phase transformation, both of which have a significant impact on fatigue life.

Using hardness based flow stress numerical model, these relationships between the processing conditions and structural parameters were further explored. Results indicated that the hard turning process design space can be partitioned into three regions based on thermal phase transformations, plastic grain refinement, and a third regime where both mechanisms are active. It was found that the Zener-Holloman parameter can not only be used to predict post-turning grain size but also to partition the process space into regions of dominant microstructural mechanisms.

Presentation IIIB-2

Materials and Processes in the Manufacture of Civil War Small Arms

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The features, performance and reliability of the Civil War era US Springfield and British Enfield rifle-muskets are briefly discussed. The “American System” of wood- and metal-working technology that enabled the mass production of military small arms with fully interchangeable parts in American and British arsenals ca. 1840-1865 is described using period illustrations. This technology is contrasted to the non-interchangeable “Craft Systems” employed in the US and Britain ca. 1800. Results of metallurgical examinations of selected components of original US Springfield and British Enfield rifle-muskets give insights to the materials, metal working processes and heat treatments available to mid-19th Century arms-makers engaged in the interchangeable "American System” of manufacture. The rifle-musket is shown to have been a value-engineered arm that employed low cost materials and metallurgical treatments, yet was capable of incredibly robust performance under combat conditions. Example antique rifle-muskets will be displayed. The life span of the muzzle-loading percussion rifle-musket in military service was short-lived – introduced in the early 1850’s, then replaced by single-shot, metallic cartridge breechloaders in the late1860’s.

Presentation IIIB-3

Low-Temperature Acetylene-Based Carburization of 316L Stainless Steel

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Low-temperature gas-phase carburization dramatically improves the hardness, wear resistance and corrosion resistance of austenitic stainless steels. However, successful application of this technology requires *in situ* removal of the spontaneously formed Cr_2O_3-rich passive film which otherwise inhibits or prevents uptake of carbon during carburization. This has previously been achieved using gaseous HCl, with it obvious negative environmental consequences. We have now demonstrated that acetylene (C_2H_2) can be used for this "activation" step. The properties of acetylene carburized 316L stainless steel will be presented. The effects of gas composition and surface microstructure of materials on the thermodynamics and kinetics of carburization will be discussed.

Presentation IIIC-1

Integrating Inelastic Light Scattering Modalities for Biomaterials Research

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The need for non-destructive analytical tools for characterizing chemical identity and mechanical properties has motivated recent instrumental and methodological innovations. Optical in elastic scattering provides a non-contact approach to physical and chemical analyses. In particular, Brillouin inelastic scattering spectroscopy can be used to determine the mechanical properties of a sample such as Young's modulus by measuring the frequency shift of the light scattered by acoustic phonons. Another inelastic scattering spectroscopy, Raman spectroscopy is widely used to provide chemical identity and to investigate conformational changes of a sample. In the work presented here, we introduce a method for simultaneously measuring the Brillouin and Raman scattered light as a means to determine both the elastic properties and chemical composition of the sample non-destructively. The primary challenge is in providing the narrow band discrimination necessary for Brillouin spectroscopy (<1 !cm-1 using 785nm illumination) and the large free spectral range needed for the Raman modality. To address this challenge, we employ a novel optical dispersive element called a virtually imaged phased array (VIPA). We have developed a numerical model of the VIPA optical response and characterized the performance of the VIPA-based imaging spectrograph. Preliminary imaging studies using the VIPA-based spectrometer are presented along with a discussion of its potential for biomaterials research.

Presentation IIIC-2

A New Multi-Technique Workstation Featuring a Plasma Ion Source

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In this presentation we will discuss the integration of a plasma-focused ion beam (FIB) into a FIB-SEM workstation. We will compare and contrast the hardware and operating principles of a plasma FIB with a liquid metal ion gun (LMIG). We will cover the most popular applications of a plasma FIB in industry and academia; the key benefits being related to the relative milling rate of a plasma FIB, which can be as much as fifty times rates practical with a LMIG. The imaging modes of the electron column will be also described, including live 3D milling (live stereo imaging) and applications of Wide Field Optics. The emergence of ToF-SIMS in combination with LMIG and plasma FIB workstations will be described as a highlight within a review of the signal detection possibilities in a FIB-SEM workstation – in both 2D and 3D data arrays.

Presentation IIIC-3

Correlating Gas Concentration Polarization with Microstructures of Porous SOFC Chathodes Using Avizo Xlab Hydro

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Solid oxide fuel cells (SOFCs) offer a method for electrochemical electricity production which can be three times more efficient than the conventional combustion engine. One of the main factors that limit SOFC performance is polarization of the porous cathode. The SOFC porous cathode is a catalyst for the reduction of oxygen. It enables the fuel cell stack to generate electricity, water and useful heat from a feedstock of oxygen on the cathode side and hydrogen on the anode side. Utilizing mixed ionic electronic conductors (MIECs) for the SOFC cathode decreases the cathodic polarization by extending the electrochemical region in three-dimensions (3D) away from the dense electrolyte/porous-cathode interface, resulting in an overall SOFC efficiency improvement.

Over the last 8 years significant progress has been made in characterizing SOFC cathodes in 3D with the use of DualBeam™ (FIB/SEM) instruments in conjunction with Avizo 3D analysis and visualization software. This study demonstrates the next step in understanding 3D porous microstructures by correlating experimentally measured cathode oxygen concentration polarization with Avizo Xlab Hydro permeability simulations. 40-60% porous La0.8Sr0.2Co0.2Fe0.8O3-δ (LSCF) MIEC cathodes were screen printed into symmetric button cells on 100 µm thick, dense yttrium-stabilized-zirconia (YSZ) electrolyte and sintered at temperatures from 850-1100 °C. Electrochemical impedance spectroscopy (EIS) was utilized to measure the cathodic polarization of these cells at 650 °C in air. The concentration polarization was measured to be between 2 and 1020 Ω, increasing with sintering temperature.
Direct simulation permeability measurements of fluid flow in 3D porous cathodes from voxelized data allow researchers to increase their R&D efficiency of microstructures with minimum resistance to gaseous flow. The commercially available Avizo Xlab Hydro solves the Stokes flow equation in order to evaluate air permeability of the above mentioned SOFC cathodes. The Avizo Xlab Hydro simulations run on 24 samples of the above LSCF cathodes resulted in oxygen permeability values between 1.3 x 10-4 d and 3.3 x 10-4 d. As expected, these permeability simulations are inversely correlated to the experimentally measured oxygen concentration polarization. This study shows that Avizo XLab Hydro is a useful tool to augment and possibly replace time-consuming benchtop permeability measurements.

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Morley Lecture

A Tale of Two Drug Candidates

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PX-866 is small-molecule analogue of the natural product wortmannin. It serves as an inhibitor of the alpha, gamma, and delta isoforms of phosphoinositide 3-kinase (PI3K) and prevents an activation of the PI3K/Akt signaling pathway. Preclinical studies have shown that PX-866 is efficacious in numerous xenograft models of human cancers, and it is currently evaluated as an anticancer agent in several Phase 1 / 2 and Phase 2 clinical studies.

XJB-5-131 is a synthetic scavenger of reactive oxygen species (ROS) in mitochondria. Mitochondria are key organelles that perform essential cellular functions and play pivotal roles in cell death and survival signaling. Hence, they represent an attractive target for drugs to treat metabolic, degenerative and hyperproliferative diseases. Shuttling organelle-specific agents or prodrugs into mitochondria holds considerable promise as an effective therapeutic strategy. XJB-5-131 has shown in vivo efficacy against hemorrhagic shock, traumatic brain injury (TBI), and age-related neurodegenerative diseases, such as Huntington's disease (HD). Related agents have also shown utility as radiation mitigators and radiation protective agents. XJB-5-131 is currently still in the preclinical development stage.

In addition to presenting these two case studies for academic drug development, this seminar will discuss the opportunities and challenges of collaborative and translational research, i.e. the goal to move findings from basic science to practical applications that enhance human health and well-being.

Poster Number One

Structure of the Catalytic Chain of *Methanococcus Jannaschii* Aspartate Transcarbamoylase in a Hexagonal Crystal Form: Insights Into the Path of Carbamoyl Phosphate to the Active Site of the Enzyme

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Crystals of the catalytic chain of *Methanococcus jannaschii* aspartate transcarbamoylase (ATCase) grew in the presence of the regulatory chain in the hexagonal space group P6322, with one monomer per asymmetric unit. This is the first time that crystals with only one monomer in the asymmetric unit have been obtained; all known structures of the catalytic subunit contain several crystallographically independent monomers. The symmetry-related chains form the staggered dimer of trimers observed in the other known structures of the catalytic subunit. The central channel of the catalytic subunit contains a sulfate ion and a K^+ ion as well as a glycerol molecule at its entrance. It is possible that it is involved in channeling carbamoyl phosphate (CP) to the active site of the enzyme. A second sulfate ion near Arg164 is near the second CP position in the wild-type *Escherichia coli* ATCase structure complexed with CP. It is suggested that this position may also be in the path that CP takes when binding to the active site in a partial diffusion process at 310 K. Additional biochemical studies of carbamoylation and the molecular organization of this enzyme in M. jannaschii will provide further insight into these points.

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Poster Number Two

RNA Splicing is a Relevant Mechanism in the Pathophysiology of Myelodysplastic Syndromes

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RNA splicing is an evolutionary mechanism important in normal protein formation. In eukaryotes, the formation of a mature and correct protein product depends on a series of biochemical reactions that includes transcription, post-transcriptional modification like conversion of immature messenger RNA (pre-mRNA) to a mature RNA, translation by ribosomes and post-translational changes. RNA splicing is the mechanism that removes regions called introns from the pre-mRNA and allows for the joining of coding regions called exons. Each step is carried out by multiprotein complexes called spliceosomes. In the last two years, RNA splicing as a pathogenetic mechanism in diseases has taken center stage in hematologic malignancies. Indeed, somatic mutations in components of the spliceosome machinery have been found in myeloid malignancies, specifically myelodysplastic syndromes (MDS) and in lymphoid cancers. MDS are a group of clonal blood diseases which lead to dysfunctional production and formation of hematopoietic cells in the bone marrow (BM) and peripheral blood (PB). Patients with MDS usually have low PB cell counts and are at risk of developing worse diseases like acute myeloid leukemia. MDS is classified in 7 categories based on morphologic and cytogenetic characteristics. *SF3B1* (splicing factor 3b subunit 1), a spliceosome component is mutated in ~68% of patients with MDS and ring sideroblasts (RS) and it has been associated with good clinical outcomes. RS is a cardinal feature of a subtype of MDS named refractory anemia with ring sideroblasts (RARS). Biologically, RS are erythroblasts with abnormal localization of iron deposition in the mitochondria which appear as a ring of blue granules under light microscopy after staining with Prussian blue. It has been reported that *SF3B1* mutant patients have down-regulation of genes important in the mitochondrial function. We investigated the biological/ clinical differences between *SF3B1* mutant and wild type (WT) patients in terms of changes in mitochondrial iron, DNA-damage, RNA-splicing, chromosomal abnormalities and methylation. We implemented two analytic technologies usually used for inorganic specimens (energy dispersive X-ray spectroscopy and electron energy loss spectroscopy) in BM cells derived from *SF3B1* mutants and WT finding more iron deposits in the mitochondria of *SF3B1* mutant compared to WT patients. In addition, the combination of these two techniques identified that ferric iron is the most prevalent form of iron carried by RS in patients with RARS; information that could not be derived by conventional Prussian blue staining. By flow cytometry, we measured the γ-H2AX, a marker of DNA-damage finding lower γ-H2AX in *SF3B1* mutants (n=8; 4.19±4.34) vs WT (n=4; 26.35±28.36). RNA-sequencing showed different splicing patterns in ribosomal proteins (RPS17). Also *SF3B1* mutants carry less chromosomal abnormalities compared to WT patients. We then found that *SF3B1* mutations are associated with genes that participate in methylation (*TET2*, *DNMT3A*), both predictors of good response to therapies. Current therapies for MDS include hypomethylating agents. *In-vitro* treatment with a hypomethylating agent, decitabine showed changes in chromatin condensation. By methylation analysis, *SF3B1* mutants have hypomethylation of genes associated with poor outcomes in MDS like *ASXL1*, *EZH2, IDH1/2, TP53,* and *RUNX1.* In sum, *SF3B1* mutant patients have more iron mitochondrial deposits, less DNA-damage and genomic instability and differences in global methylation. Altogether these biological features might explain the better clinical outcomes of *SF3B1* mutant patients.

Poster Number Three

Adenovirus Immunity: Insights from Coagulation Factor VII on How X Marks the Spot

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Adenoviruses (Ads) are promising as vectors for gene therapy based on their ability to accommodate relatively large transgenes and efficiently infect several human cell types with high levels of gene expression. However, a limitation to using the Ad-based delivery system is that upon intravascular injection several vitamin K-dependent blood coagulation factors can form a complex with the hexon protein of the adenoviral capsid, which contributes to virus sequestration in the liver by facilitating transduction of hepatocytes. Coagulation factors FVII and FX bind human adenovirus species C type 5 (HAdv5) hexon with very high affinity, but only FX appears to play a role in mediating selective uptake of Ad into the liver. To understand the lack of effect of FVII on supporting Ad cell entry, we undertook a cryo-electron microscopy (cryo-EM) structural study of the HAdv5-FVII complex. A subnanometer resolution cryo-EM structure was analyzed using guided molecular dynamics simulations. Results indicate that FVII binds within the HAdv5 hexon in a different orientation than previously observed for FX, although several of the same hexon residues are involved (T423-E424-T425). In addition, we found that when bound to hexon, two proximal FVII molecules interact via their serine protease (SP) domains and bury potential sulfate proteoglycan receptor binding residues within the dimer interface. Several HAdv5 hexon mutants were generated and examined in the presence of FVII, one of which (T425A) completely abrogated FVII binding. Mutating HAdv5 residues T423G-E424A at the hexon-FVII GLA interface resulted in superior cell transduction efficacy in the presence of FVII. Molecular dynamics simulations of FVII binding to the T423G-E424A hexon mutant revealed an altered interface that could affect the orientation of FVII as well as SP domain dimer formation. Our data suggests that when FVII binds to virions with the hexon T423G-E424A mutations FVII adopts a different orientation relative to the viral capsid, SP domain dimer formation is prevented, and this allows highly effective virus-mediated gene transfer. In summary, this structural and biochemical study revealed the important role of HAdv5 hexon residues (T423-E424-T425) in interaction with FVII and FX and their impact on hepatocyte infectivity.

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Poster Number Four

Low-Temperature Acetylene-Based Carburization of 316L Austenitic Stainless Steel

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Low-temperature gas phase carburization dramatically improves the hardness, wear resistance and corrosion resistance of austenitic stainless steels. However, successful application of this technology requires *in situ* removal of the spontaneously formed Cr_2O_3-rich passive film which otherwise inhibits or prevents uptake of carbon during carburization. This has previously been achieved using gaseous HCl, with its obvious negative environmental consequences. We have now demonstrated that acetylene (C_2H_2) can be used for this "activation" step. The effects of microstructure, time and gas composition on the thermodynamics and kinetics of acetylene-based carburization will be discussed, as well as the properties of such interstitially hardened stainless steel.

Poster Number Five

An Automatic Additive and Multiplicative Noise Removal Scheme with Sharpness Preservation

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To remove noise from biomedical images polluted by excessive and inhomogeneous additive or multiplicative noise, most of the denoising algorithms cannot keep a desirable balance between denoising and preservation of fine features; only work for one specific noise; and involve heuristic parameter tuning. We present a fully automatic approach to preserve sharp edges and fine details while removing noise. Explained in nonlocal means scheme, we propose a segmentation boosted NL-means filter (SNL) based on the concept of mutual position function to ensure averaging is only taken over pixels in the same phase. To address unreliable segmentation due to excessive noise, we apply SNL filtering in an iterative way. Comparison with ROF, BM3D, K-SVD and the original NL-means on simulated data, MRI and SEM images indicates potentials of our method.

Poster Number Six

The Effect of Minor Alloying Additions of Cr and/or Pt on the Microstructure of the Oxide/Metal Interface of Ni36Al after Hot Corrosion Exposure

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Our work has surveyed the structure of the oxide/metal interface minor element additions of Cr and/or Pt using transmission electron microscopy (TEM). All compositions studied are based on Ni-36Al after 20 hours of hot corrosion exposure at 700˚C with an atmosphere containing 1000ppm SO_2. TEM foils were prepared using focused ion beam (FIB) milling.

The addition of either 5 at % Cr or 5 at % Pt significantly improves the hot corrosion resistance of the Ni-36Al alloy, though it appears that the mechanism of the improvement is different. The addition of both 5Cr and 5Pt in the same time restores the poor hot corrosion resistance. The mechanism by which these improvements occur is under study. Significant differences are seen in the microstructure of the metal near the oxide/metal interface. The smallest reaction zone was on the alloy with just 5Cr added, which formed a 1µm thick layer of a γ' phase underneath the oxide. All of the other samples had larger transformation zones. We believe this behavior has a significant effect on the long-term hot corrosion resistance of these alloys and further work is assessing the importance of the transformation during hot corrosion.

Poster Number Seven

The Effect of Prior Exposures on the Notched Fatigue Behavior of Disk Superalloy ME3

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For gas turbine disks, some effects of service may be captured by extended exposures at elevated temperatures prior to conventional fatigue testing. Oxidation at potential service conditions (704-815 °C up to 2,020 hours) and its effects on notched fatigue behavior for disk superalloy ME3 was examined. Oxidation produces an external scale, subscale that extends into a γ'-dissolution layer, and dissolution of grain boundary carbides through and beyond these layers. Pronounced fatigue debits were driven by this surface damage and increased with damage depth. Irrespective of exposure temperature, exposures that produced roughly equivalent surface attack resulted in statistically equivalent fatigue lives. Surface crack initiations shifted with increasing exposure from predominately single initiations with transgranular propagation to multiple initiations from the cracked external oxide with intergranular propagation. Testing and characterization was performed to ascertain the origin of the intergranular propagation, including chemical evaluation of affected grain boundaries with atom probe tomography.

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Poster Number Eight

Application of Focused Ion Beam (FIB) Instrumentation in Preparation of Cross-Sections of Materials

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Focused Ion Beam (FIB) instrumentation is used to prepare cross-sections of materials for examination in Scanning Electron Microscopy (SEM). Gallium ions are used to mill the material with different beam conditions used to fine polish the cross section. This technique preserves the material structure better compared to mechanical polishing methods using SIC paper and polishing compounds. Several examples will be shown.

Poster Number Nine

Synthesis and Characterization of Indium Gallium Molybdate $Ga_{2-x}In_xMo_3O_{12}$

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Negative thermal expansion (NTE) materials are compounds that reversibly shrink when heated. Such materials have a range of potential applications in dentistry, ceramics, or electronics as an additive to polymers. A composite made with an NTE material could be used to improve durability and lifetime for applications. Several families of NTE materials exist, one of which is the $A_2M_3O_{12}$ family in which A is a trivalent cation and M is molybdenum or tungsten. A new material is being investigated, in which A is indium and gallium ($InGaMo_3O_{12}$). It can be synthesized using the non-hydrolytic sol-gel (NHSG) technique, and the optimum parameters of its synthesis are being determined to obtain phase pure, homogenous material. With certain reaction conditions, crystallization at very low temperatures has been observed. Samples are characterized using powder x-ray diffraction (PXRD), thermogravimetric analysis (TGA), and scanning electron microscopy (SEM) in combination with energy-dispersive spectroscopy (EDX).

Poster Number Ten

Microstructure Change of SOFC Anode During Long-Term Operation Evaluated Using 3D Reconstruction

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Changes in the microstructure of an anode in a solid oxide fuel cell (SOFC) stack have been studied using focused-ion-beam sectioning and 3D reconstruction of scanning electron microscope images. The SOFC had been operated at 925 °C for 8500 h. The three phases of the anode — the metallic Ni electronic conductor, the ceramic yttria-stabilized zirconia (YSZ) ionic conductor, and the pore phase crucial to the density of the three-phase boundaries — were characterized using volume fraction of each phase, particle diameters, tortuosity and surface area. Significant changes in the anode microstructure were detected.

Poster Number Eleven

Inhibition of Mitochondrial Fission: A Potential Neurodegenerative Therapy

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Mitochondria are essential organelles involved in the generation of chemical energy, maintenance of calcium levels and induction of apoptosis. Therefore, understanding the complete function and behavior of these organelles is an important area of research. Mitochondria undergo cycles of fission and fusion that regulate mitochondrial content exchange, mitochondrial shape control, mitochondrial communication with the cytosol and mitochondrial quality control. Excessive fusion results in collapsed interconnected mitochondrial networks, and excessive fission produces fragmented organelles. Excessive fission is also linked with aging, neurodegeneration and apoptosis. The protein responsible for mitochondrial fission in mammals is dynamin-related protein 1 (Drp1). Drp1 is a dynamin like GTPase that exists as a tetramer in solution, and is capable of forming large oligomers that constrict the outer mitochondrial membrane to mediate membrane scission. Using electron microscopy, I have observed Drp1 tubulation around liposomes. Drp1 can also tubulate in the presence of GTP. My goal is to understand structurally and mechanistically how Drp1 oligomerizes using electron microscopy and computational methods. In addition, we also believe that Drp1 can be influenced by post-translational modifications, such as oxidation. In the presence of a cysteine specific oxidizing agent, Drp1 forms larger oligomers which may also play a role in regulating mitochondrial fission. Many neurodegenerative diseases such as Parkinson's, Alzheimer's and Huntington's all display increased drp1 fission activity, leading to increased cell death and neurodegeneration. As a potential therapy for these diseases, I am testing the effect of Drp1 inhibitory peptides. By inhibiting increased mitochondrial fission in neuronal tissues, many of these devastating neurodegenerative diseases could potentially be treated.

Poster Number Twelve

Characterization of the Chain-Ends, Backbone and Branching Structures in Polyvinylidene Fluoride with T1 and 2D DOSY NMR Techniques

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The structures of backbone, branch and chain-end fragments have a strong influence on the physical and chemical behavior of polymers. In this work, the chain-end units in PVDF (Polyvinylidene fluoride) were identified with two different methods: spin-lattice relaxation experiments (T_1 measurements) and Diffusion Ordered Spectroscopy (DOSY) NMR experiments. Spin-lattice relaxation experiments measure the recovery rate of the nucleus' magnetization on z direction (B_0) to its equilibrium value. Since the atoms from the chain-end of the polymer have faster motion, they have a relatively longer T_1's compared to those of atoms from the backbone and branches. 2D DOSY measures diffusion rates, which are mostly based on the molecular size. The diffusion rate of chain-end structures in a polymer is faster than that of backbone structures because on average most chain ends are from low molecular weight molecules, whereas most backbone units are in high molecular weight molecules. The combination of T_1 and 2D DOSY experiments can provide solid evidence for identifying NMR resonances of chain ends and short chain branches in polymers.

Poster Number Thirteen

A Critical Role of Electron Microscopic Examination in Diagnosis of a Deciduoid Mesothelioma Case

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Deciduoid mesothelioma is a rare malignant disease with poor prognosis. It is often misdiagnosed as peritoneal deciduosis, mesothelial hyperplasia, or metastatic malignancy[1]. Differential diagnosis is critical because ectopic dedidua does not require aggressive treatment[2] and specific therapeutic choices would be indicated when metastatic malignancy is confirmed. Here we report a case of peritoneal deciduoid mesothelioma diagnosed through histological, immunological and ultrastructual examination. Multiple tumor masses in pelvis were detected by MRI in a 40-year-old woman who complained intermittent abdominal pain over a month. Initial routine analysis of the tumor debulking specimen indicated differential diagnosis of melanoma mesothelioma, and poorly differentiated carcinoma. HE staining detected eosinophilic cuboid stroma cells resembling deciduas. Immunostaings were positive for cytokeratin 5/6, WT1, and calretinin. Electronmicroscopy detected slender and long microvilli, a characteristic of mesothelial differentiation morphology. All these findings confirmed the case was deciduoid mesothelioma.

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Poster Number Fourteen

Raman Chemical Imaging of Poly-L-Lactide Bioimplants Using an Acoustio-Optic Tunable Filter

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Poly-L-lactide (PLLA) is a biodegradable and biocompatible implant polymer that can be endowed with varying degrees of elasticity and piezoelectricity depending on the extent of its long-range molecular order. In its amorphous state, PLLA exhibits no net piezoelectric response. Cold-drawing PLLA at temperatures above the glass-transition temperature and below the cold crystallization temperature induces molecular ordering. As the draw ratio increases, corresponding increases in the piezoelectric properties and degree of crystallinity are observed. At draw ratios greater than 4.5, fibrillization begins to dominate and these molecular order-induced properties diminish. By tailoring the crystallinity of PLLA, its degradation rate, Young's modulus, and piezoelectricity can be enhanced for a particular application in vivo.
In the work presented here, we have developed a wide-field Raman imaging system based on a narrow passband acousto-optic tunable filter. Our implementation overcomes some of the current limitations of AOTF imaging systems and combines novel multivariate strategies with AOTF-based acquisition to provide high resolution images of crystalline content. The multivariate method employs a new Gram-Schmidt orthogonalization method to establish a reference spectrum for automated image analysis based on spectral correlation. A full theoretical treatment of the multivariate approach and the design of the novel wide-field AOTF Raman imaging system are presented.

Poster Number Fifteen

Effects of Composition Changes on Mechanical Properties of Iron-Based Metallic Glass Ribbons

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Vickers micro-hardness, tension tests, notch and fatigue precrack toughness tests, as well as controlled monotonic and cyclic strain experiments via bending over mandrels of different diameter have been performed on two different chemistries of Fe-based (Fe-Si-B) metallic glass ribbons. Tensile strengths of $Fe_{73.5}Cu_1Nb_3Si_{13.5}B_9$ were 2000 ±100 MPa and 1640 ±35 MPa for $Fe_{78}Si_9B_{13}$, consistent with the micro-hardness trends. High notch toughnesses (e.g. 89 ±0.9 $MPam^{1/2}$ - $Fe_{73.5}Cu_1Nb_3Si_{13.5}B_9$; 94.5 ±5.5 $MPam^{1/2}$ - $Fe_{78}Si_9B_{13}$) and fatigue precracked toughness of 76 $MPam^{1/2}$ for the $Fe_{73.5}Cu_1Nb_3Si_{13.5}B_9$ and 80 $MPam^{1/2}$ for the $Fe_{78}Si_9B_{13}$ were obtained. Flex bending cyclic fatigue tests revealed a fatigue limit of 385 MPa for $Fe_{78}Si_9B_{13}$ ribbons, while the more brittle behavior of the $Fe_{73.5}Cu_1Nb_3Si_{13.5}B_9$ ribbons prevented generation of flex bending fatigue data. SEM examination was used to characterize all fracture surface details. These results are discussed in the light of recent work on metallic glass systems.

Poster Number Sixteen

Mechanical Behavior of Nano-Structured Aluminum Composites

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The mechanical behavior of nano-structured aluminum composites was determined in tension, toughness, and fatigue at temperatures ranging from room temperature to 260°C. The materials were produced by extrusion of amorphous aluminum powders to create a nano-structured aluminum composite with high volume fraction of reinforcement. The resulting material exhibited high strength and excellent high cycle fatigue resistance over a range of test temperatures relevant to high temperature aluminum alloys. The effects of creating a nano-structured composite on the balance of properties will be summarized, along with laminated versions.

Poster Number Seventeen

Toward the Purification of Ornithine Transcarbamoylase from *Methanococcus Jannaschii*

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Ornithine Transcarbamylase (OTCase) is an enzyme used to catalyze the reaction of ornithine and carbamoyl phosphate to produce citrulline and phosphate. OTCase can be found in the process of arginine biosynthesis in plants and microbes and has a role in the urea cycle of mammals. A genetic OTC deficiency in humans is a urea cycle disorder that results in hyperammonemia. OTCase belongs to the transcarbamoylase family of proteins and has similarities in sequence and structure with aspartate transcarbamoylase (ATCase). In both enzymes, the catalytic subunit contains two domains, the N-terminal or CP-binding domain and the C-terminal or aspartate/ornithine binding domain.

We have been working with the OTCase from the hyperthermophilic archaeon *Methanococcus jannaschii* and are trying to develop a successful strategy for its purification. To this end, a heat step at 60° C and DEAE anion exchange chromatography appear promising steps. In the poster, we will show our work up to this point. Using the colorimetric assay, we have confirmed that our preparation contains the enzyme and that it follows Michaelis Menten kinetics.

Poster Number Eighteen

Low-Temperature Gas-Phase Paraequilibrium Nitridation of Duplex Stainless Steel 2205

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In an effort to increase the desirable properties (hardness, wear-, fatigue-, and corrosion-resistance) of duplex (ferrite + austenite) stainless steel 2205, the material was subjected to a low-temperature gas-nitriding heat treatment similar to the established Swagelok carburization process, which is commercially utilized for such improvements of austenitic stainless steels. CALPHAD-based thermodynamic modeling was first used to predict the (i) paraequilibrium solubility of nitrogen and (ii) transformations that may occur in both the austenitic and ferritic phases during the isothermal heat treatment and concomitant dissolution of nitrogen. Treated samples were then characterized via XRD, SEM, EBSD, AES, and TEM to determine the chemistry and microstructure of the hardened layer. Austenitic grains behaved similarly to those in purely austenitic stainless steel: a precipitate-free, highly supersaturated 'expanded-austenite' case was formed. The most enlightening result was the fine microstructural details present in the formerly ferritic grains. Detailed structural and analytical characterization conducted in the TEM revealed a high-nitrogen 'bcc-like' phase, and a highly defective, low-symmetry phase heretofore not found in the (Fe,Cr,Ni)-N systems. The treated samples exhibited unattenuated or improved pitting corrosion resistance over non-treated material, depending on the treatment parameters used.

Poster Number Nineteen

Circulating Blood-Derived Phagocytes not Microglia are Responsible For Axonal Die Back after Spinal Cord Injury

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The size of a traumatic spinal cord injury increases over the first few weeks and axons die away from the center of the lesion. Axonal dieback occurs by two mechanisms: an initial phase of dieback occurring over several hours, and a secondary, inflammatory, phase that takes place over the first few weeks after injury. The secondary period after injury has long been correlated with macrophage infiltration (Busch 2009 J Neurosci 29:9967–9976). Here, we propose a cellular mechanism for this inflammatory phase of dieback. Using powerful time lapse multi-photon imaging, we imaged interactions between immune cells and axons in a mouse dorsal column crush spinal cord injury model. Individual axons were identified by yellow fluorescent protein expressed in a neuronally restricted manner under the Thy-1 promoter (Feng 2000 Neuron 28(1):41-51). CX3CR1-positive monocytes and microglia were identified by green fluorescent protein expressed under of the CX3CR1 promoter (Jung et al. 2000 Mol Cell Biol 20(11):4106-14). Utilizing a radiation chimeric model in which marrow-derived cells CX3CR1 positive cells can be distinguished from radio-resistant CNS CX3CR1 positive resident microglial cells, we determined that the vast majority of the CX3CR1-positive cells within the lesion are derived from the blood instead of from resident microglia. In the first week after injury, axonal retraction bulbs are static except when axonal bits are lost by a blebbing mechanism in response to physical contact followed by phagocytosis by CX3CR1-positive cells derived from the blood. All observed destructive events took place in response to contact by a blood derived CX3CR1 positive macrophage, not resident microglia. Understanding the *in vivo* cellular interactions involved in this secondary axonal injury may lead to clinical treatment candidates that involve modulation of infiltrating blood monocytes.

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Poster Number Twenty

New Method for Analyzing the Surface Chemistry of Copper Oxide

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Samples of copper (II) oxide were tested to determine the composition of the chemically active surface compared to the bulk. Copper, manganese, and zinc concentrations were quantified through external standardization, after dissolution with nitric acid using High Performance Liquid Chromatography (HPLC) and Atomic Absorbance Spectroscopy (AAS). The change in the ratios of zinc and manganese to copper demonstrated the reactivity at different depths of the copper oxide powder sample. The study shows that there is larger zinc to copper ratios on the surface of the powder in comparison to the bulk. Trends also suggest that the manganese-to-copper ratios steadily increases as the powder is dissolved. Further analysis showed that particle size was a significant factor in surface composition of zinc and manganese. The smaller particle size showed a higher ratio of zinc and manganese-to-copper. Further investigation is necessary to confirm these trends.

Poster Number Twenty One

Removing Angular Symmetry in Spectral Angle-Based Hyperspectral Image Analyses

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The efficacy of hyperspectral image segmentation is strongly reliant on the limitations of pixel-wise classification methods, most of which are based on chemometric strategies that do not account for spatially dependent variations across the image field of view. Spatial inhomogeneity arises from a variety of causes including non-uniform sample illumination and unequal optical coupling efficiencies between axial and off-axis rays in the image path. These inconsistencies are often manifested in the data as variations in the signal to noise ratio across the image field. In the work presented here, we describe a novel method of hyperspectral image classification based on spectral angle and spectral vector pointing stability that reduces the misclassification frequency. We provide a theoretical framework upon which the accuracy of the classified image can be estimated without a priori information about the spatially dependent variations. In addition, we demonstrate the utility of the method on both modeled hyperspectral image data and Raman hyperspectral data obtained for cold-drawn poly-L-lactide.

Poster Number Twenty Two

Isolation and Characterization of a Suspected Phytoalexin from *Acer rubrum* L

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Wilted red maple leaves are toxic to horses, causing death by oxidation of hemoglobin and inducing anemia. Gallic acid derivatives have been identified as the main oxidants present in the leaves. However, our work has found that a previously unknown phytoalexin is produced by wilting red maple leaves. Phytoalexins are defensive compounds produced by plants in response to fungal attack, and these compounds often have a range of biological activities. The compound, which fluoresces blue in certain TLC systems, is present only after wilting. The objective of this study is to identify and characterize this compound so that its toxicity can be determined. Wilted leaves were collected, dried, and extracted with methanol. Leaf extracts have been purified through repeated thin layer chromatography column chromatography, and preparative HPLC. After successful purification, the structure of the compound will be confirmed by NMR and mass spectral analysis. This research will provide insight regarding the mechanism of fungal defense in *Acer rubrum* and may also be relevant to the known toxicity of wilted red maple leaves to horses.