2017 RESEARCH HIGHLIGHTS

CHEMICAL ENGINEERING & MATERIALS SCIENCE

MICHIGAN STATE UNIVERSITY

COLLEGE OF ENGINEERING

FROM THE CHAIR

This past academic year has been one of continued growth for the department and its research and teaching programs. Several new faculty, teaching specialists, and staff have joined the ranks, and the department administrative office has moved into more functional space in the Engineering Building. We are proud to continue to strengthen our research efforts in chemical engineering and materials science and enhance the delivery of education in these fields to our students. It has been a busy year, and I am delighted to present a few of the highlights to you here.

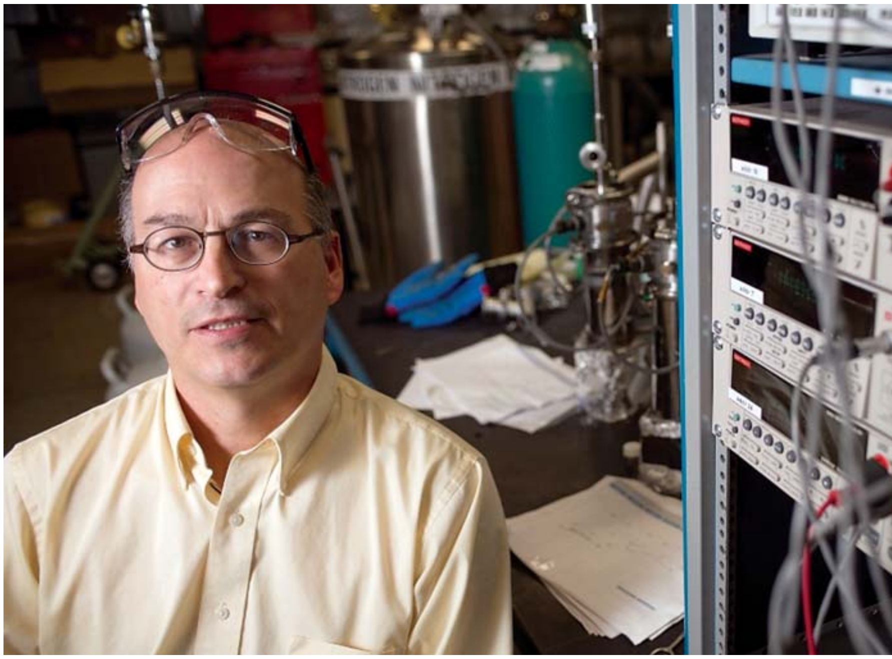
LAMP ENDOWED CHAIR IN CHEMICAL ENGINEERING

We are very pleased to announce that **John Dorgan**, previously Professor in the Department of Chemical and Biological Engineering at the Colorado School of Mines, has been named the David and Denise Lamp Endowed Chair in Chemical Engineering. John brings to ChEMS a wealth of expertise and experience in the area of polymers, composites, and biomaterials for energy and sustainability applications, and we look forward to his leadership in these research areas as well as contributing to our instructional programs. Welcome John!

OTHER NEW FACES IN CHEMS

In addition to the Lamp Chair, the department is delighted to have added several new faculty and staff to both the chemical engineering and materials science programs:

- **Alexandra Zevalkink** joined ChEMS in August as assistant professor, adding strength to our programs in energy materials.
- In January, **Xanthippi Chatzistavrou** joined the department as assistant professor. Her research interests are in the area of glass-ceramic composites for biomedical applications.
- **Steve Kamin**, who brings over 30 years of industrial experience in chemical engineering process and design, joined ChEMS in January as a teaching specialist in the chemical engineering program.
- Finally, the department is very happy to welcome a new graduate secretary, **Tiffany Owen**.



OUTSTANDING FACULTY AND STAFF CONTINUE TO WIN AWARDS AND HONORS

In the past year, numerous faculty members have distinguished themselves through prestigious awards and honors:

- **Larry Drzal** was honored with two national awards: the Medal of Excellence in Composite Materials from the University of Delaware, and the Lifetime Achievement Award from the Automotive Division of the Society of Plastics Engineers.
- **Bobby Bringi**, research professor and former CEO of MBI, was inducted into the American Institute for Medical and Biological Engineering (AIMBE) College of Fellows.
- **K. Jayaraman** was named a Fulbright Scholar, and his visiting appointment at the Karlsruhe Institute of Technology began March 1.
- **Tom Bieler** received the ASM Henry Marion Howe Medal for best paper in *Metallurgical and Materials Transactions*.
- Last May, **Martin Hawley** was honored with the 2016 Claud Erickson Award, the highest honor presented to a graduate by the MSU College of Engineering.
- **Nathan Mellott**, teaching specialist in materials science, was awarded the department's 2017 Withrow Teaching Excellence Award.
- Administrative assistant **Jennifer Keddle** was recognized with the Gloria Stragier Award for Dedicated and Creative Service at the Withrow ceremony in March.
- **Wei Lai** was promoted to associate professor with tenure, and **Richard Lunt** was promoted to associate professor with tenure and appointed to the Johansen Crosby Chair in Chemical Engineering.
- **Yue Qi** was a recipient of the Brimacombe Medal from the TMS Society for her work on lithium ion batteries.

HIGH-ACHIEVING STUDENTS

- **Rebecca Carlson**, who will graduate in May with a degree in chemical engineering, was awarded a National Science Foundation Research Fellowship in 2017.
- **Rebecca** was also named a Hertz Foundation Fellow, and she will begin her graduate studies in bioengineering at MIT.
- **Rebecca** and 2016 MSU chemical engineering graduate **Ariel Rose** won first place in the 2016 AICHE Student Team Design competition.
- 2016 graduate **Rebecca Jacobs** received first place in the AICHE Safety in Design competition.
- **Joshua Young**, a junior in the materials science and engineering program, received a $15,000 scholarship from the Elwood Group in March.

DISTINGUISHED ALUMNUS

In May, the 2017 Red Cedar Circle Distinguished Alumni Award will be presented to outstanding ChEMS alumnus **Joe Lin**, President of Diotec Electronics Corporation

As you can see from these activities and accomplishments, our faculty, staff, and students continue to excel in carrying out our mission of excellence in research, teaching, and service. The research highlights presented in this publication are further testament to the commitment of our faculty to advance knowledge and understanding in chemical engineering and materials science. I hope you enjoy reading about them.

DONALD MORELLI, *Interim Chair and Professor*

DEPARTMENT HIGHLIGHTS

The Michigan State University Department of Chemical Engineering and Materials Science (ChEMS) has vibrant research programs in both chemical engineering and materials science and engineering.

OUTSTANDING FACULTY

Among our 31 faculty members, we have:

- Six NSF CAREER Award winners
- Four University Distinguished Professors
- Four MSU Distinguished Faculty/William J. Beal Outstanding Faculty winners
- Two MSU Teacher-Scholar Award winners
- Four Withrow Distinguished Scholar Award winners
- Eight Withrow Teaching Excellence Award winners (several have won multiple times)

Also included among the faculty ranks are multiple society Fellows:

- National Academy of Inventors
- American Institute of Chemical Engineers
- American Institute of Chemists
- American Institute for Medical and Biological Engineering
- Society of Plastics Engineers
- ASTM International
- American Ceramic Society
- ASM International
- ABET
- American Physical Society

Many faculty members have also received national and international recognition for their academic and research achievements.

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DEPARTMENT ACHIEVEMENTS

- Total research expenditures are about $9 million annually
- Approximately 130 refereed publications and 9 patents per year
- Growth of the total undergraduate student population to 799 (as of Fall 2016)
- Graduate enrollments of 87 PhD students and 11 MS students (as of Fall 2016)

RESEARCH CENTERS

The department operates a number of major research centers, including:

- the Composite Materials and Structures Center

and two Department of Energy (DOE)-funded centers:

- Great Lakes Bioenergy Research Center
- the light-and-heavy-duty vehicle component of the Institute for Advanced Composites Manufacturing Innovation (IACMI)

A NATIONAL CENTER OF EXCELLENCE

To support our mission of being nationally recognized as a center of excellence in research, teaching, and service, four goals have been targeted:

- Provide leadership and excellence in conducting nationally recognized, innovative, and cutting-edge research
- Recruit high-performing students and deliver modern, high-quality graduate and undergraduate programs that produce top-notch graduates serving the needs of industry, government, and academia
- Offer outstanding professional and outreach services
- Conduct fundraising from the private sector, state, and federal sources, and provide stewardship in support of research, instruction, and service

STRATEGIC INITIATIVES

As we look to the future, the department has established strategic initiatives to ensure our continued ascension in productivity and prominence:

- Continued faculty growth to complement and supplement our research priorities
- Recruitment of a growing pool of high-quality PhD students
- Increased recruitment of highly qualified undergraduate students, and matriculation of bachelor's degree graduates that are prepared to solve the problems of both today and tomorrow
- Enhanced support of endowments for fellowships, scholarships, professorships, and the discretionary excellence fund

The department has positioned itself and established its research priorities to address critical 21st-century challenges such as energy and sustainability, nanotechnology and materials, and biotechnology and biomedical engineering.

FACULTY BIOS

KRIS BERGLUND (PG. 1)

Kris Berglund is an MSU University Distinguished Professor of Food Science and Chemical Engineering with joint appointments in the Department of Chemical Engineering and Materials Science, and the Department of Food Science and Human Nutrition. He received an MS degree from Colorado State University in 1980 and a PhD from Iowa State University in 1981. His research is on new and alternative uses of agricultural and forest raw materials; and separation, purification, and crystallization processes for food, pharmaceutical, and chemical industries. He is also focused on distilled beverage technology. He founded and has run the school's Artisan Distilling Program since 1996. Recently, with his efforts, a minor in Beverage Science and Technology was made available to MSU students beginning in the fall of 2013.

THOMAS BIELER (PP. 2–3)

Thomas R. Bieler is a professor in the Department of Chemical Engineering and Materials Science, and a researcher in the Composite Materials and Structures Center. He received his BA in Applied Mechanics at University of California at San Diego in 1978 followed by a MS in Ceramic Engineering at University of Washington (Seattle) in 1980. He worked for five years at Sandia National Laboratory in Livermore on high-rate deformation. He completed his PhD in materials science (with a minor in continuum mechanics) at University of California–Davis in 1989, and has been at Michigan State University thereafter. His research focuses on characterization of mesoscale deformation mechanisms and plasticity modeling in titanium-based alloys, tin in the context of lead-free solder joints, and high-purity niobium used in superconducting particle accelerator cavities. With colleagues, he has published 270 papers, 34 of which have been cited more than 34 times. He was awarded the Distinguished Scientist/Engineer and the Service Award in the Materials Processing and Manufacturing Division of the Mining, Metallurgical and Materials Society (TMS) in 2013.

■ CARL BOEHLERT (PP. 4–5)

Carl Boehlert is a professor in the Department of Chemical Engineering and Materials Science. He received a BS degree in Agricultural and Biological Engineering from Cornell University in 1991, followed by both an MS and PhD in Materials Science and Engineering at the University of Dayton, in 1993 and 1997 respectively. He worked in the Johns Hopkins University Department of Mechanical Engineering and the Nuclear Materials Technology Division of Los Alamos National Laboratory before coming to Michigan State University in 2005. His research interests include materials engineering; materials sciences; metallurgy; electron backscatter diffraction; intermetallics electron microscopy; metal matrix composites; titanium alloys and composites; mechanical behavior. His research group is concentrating on understanding the deformation behavior of hexagonal close-packed metals, in particular, titanium and magnesium alloys, under extreme environments. He is a past winner of both the Department of Engineering (DOE) PECASE and National Science Foundation (NSF) Career Awards.

■ DAINA BRIEDIS

Daina Briedis is an associate professor in the Department of Chemical Engineering and Materials Science, and assistant dean for Student Advancement and Program Assessment in the MSU College of Engineering. She has been involved in several areas of discipline-based education research (DBER) including student retention, curriculum redesign, use of technology in the classroom, and understanding of engineering identity. She helps facilitate student success through evidence-based improvement processes both at the college and the program level. She has been a co-PI on two NSF grants in the areas of integration of computation in engineering curricula and in developing comprehensive strategies to retain early engineering students. Dr. Briedis is active nationally and internationally in engineering accreditation, serving as Adjunct Director of Professional Development at ABET and facilitating ABET assessment workshops and Program Evaluator Training. She is a Fellow of ABET, ASEE, and AIChE. Her hobbies include cross-country skiing, hiking, and water skiing, and she is an avid football fan. When she has time, she enjoys reading, cooking, and gardening.

■ SCOTT CALABRESE BARTON (PP. 6–7)

Scott Calabrese Barton is an associate professor in the Department of Chemical Engineering and Materials Science. His research concerns electrochemical engineering with a focus in catalysis and transport in electrochemical energy systems, from experimental and theoretical perspectives. Electrochemistry dramatically impacts numerous technologies for energy and chemical production, including modern electric and hybrid vehicles. A key enabler of these technologies are electrocatalysts. Dr. Barton's research group studies new electrocatalysts, materials, and electrode design for fuel cells and chemical conversion. Transition metal electrocatalysts are being studied as replacements for high-cost platinum, and could potentially lower the cost of fuel cell systems and enable practical fuel cell vehicles. Bioconversion involving enzyme electrocatalysts may lead to conversion of renewable resources to value-added chemicals. Professor Barton's group is developing electrodes to achieve such bioconversion, including catalysts for regeneration of enzyme cofactors, and high-surface carbon materials for immobilization of enzymes, catalysts, and cofactors. Throughout this work, mathematical models are incorporated to build understanding of electrochemical kinetics and transport, leading to tools for analysis and optimization of novel electrode architectures. He received his PhD in chemical engineering from Columbia University in 1999, after studying aerospace engineering at Notre Dame and MIT. He is the recipient of a prestigious CAREER award from the National Science Foundation and a Petroleum Research Fund award from the American Chemical Society.

■ CHRISTINA CHAN (PP. 8–9)

Christina Chan is the George W. Bissell Professor of Chemical Engineering at Michigan State University. In addition to her appointment in the Department of Chemical Engineering and Materials Science, she has joint appointments in the departments of Biochemistry and Molecular Biology, and Computer Science and Engineering. Dr. Chan is pioneering work at the interface of biology, chemistry and chemical engineering, and computer science and engineering, leading an integrative approach to the study of medical and biological problems. Her research focuses on bioinformatics and functional genomics as well as cellular and molecular engineering to analyze cellular processes and disease mechanisms. Her work on exploring the mechanisms by which elevated levels of free fatty acids mediate abnormalities in cellular function and metabolism that contribute to the development of severe chronic diseases, such as obesity, cancer and Alzheimer's disease, is groundbreaking. Precision medicine is an emerging approach for treating complex diseases by taking into account the variability in genes and environment of each individual. The Chan laboratory takes a systems approach to understanding how molecular and environmental events influence one another as parts of an overall system, and together provides information that can improve the precision with which patients are categorized and treated. Dr. Chan has been recognized for her many research and academic contributions, including the Whitaker Young

Investigator Award (2003–2006), the College of Engineering College of Engineering Excellence in Teaching Award (2010), Engineering's College of Fellows (2012), and the MSU William J. Beal Outstanding Faculty Award (2014). She was elected as a Fellow of the American Institute of Medical and Biological Engineering in 2011. She received her MS (1986) and PhD (1990) in chemical and biochemical engineering from the University of Pennsylvania.

XANTHIPPI CHATZISTAVROU (PP. 10–11)

Xanthippi Chatzistavrou is an assistant professor in the Department of Chemical Engineering and Materials Science with research interests in the field of biomaterials and tissue engineering. Her expertise is on sol-gel derived bioactive glasses and glass ceramics with antibacterial properties for combating antibiotic-resistant bacteria with applications in dentistry and orthopedics. Her research work includes micro- and nano-size bioactive particles with dual antibacterial action based on the delivery of heavy metals and antibiotics. Antibacterial coatings and scaffolds capable of healing and regenerating hard and soft tissue. Composites with natural and synthetic hydrogels that will be used as biomimetic injectable vehicles for the delivery of antibacterial and bioactive agents to combat osteomyelitis and periodontitis or peri-implantitis. Dr. Chatzistavrou focused her interest in solid state physics and materials science, after obtaining a comprehensive background in physics. She did her Master's degree and PhD studies in the Department of Physics at the Aristotle University of Thessaloniki in Greece. After her graduation she was awarded some of the most prestigious fellowships for individual young scientists in Europe and Japan. These fellowships gave her the opportunity to work as a postdoctoral researcher in some of the top Departments and Institutions in Materials Science worldwide (Imperial College, UK; University of Erlangen-Nuremberg, Germany; Nagoya Institute of Technology, Japan). Prior to joining MSU and the Department of Chemical Engineering and Materials Science in 2017 she was appointed as a Research Fellow in the School of Dentistry at the University of Michigan. She has published more than 40 peer-reviewed papers. She has contributed as a co-author in four book chapters and delivered more than 30 presentations both oral and in poster form at international conferences.

MARTIN A. CRIMP (PP. 12–13)

Martin A. Crimp is a professor in the Department of Chemical Engineering and Materials Science, and a researcher in the Composite Materials and Structures Center. He received BS (1981) and MS (1984) degrees in metallurgical engineering from Michigan Technological University and a PhD (1987) in materials engineering from Case Western Reserve University. After carrying out postdoctoral research in the Department of Metallurgy and Science of Materials at the University of Oxford, he joined the MSU faculty in the Department of Metallurgy, Mechanics, and Materials Science (1989). He has since risen to the rank of professor in the Department of Chemical Engineering and Materials Science. He applies a wide range of diffraction based electron microscopy techniques to a variety of materials problems. Of particular note he has been at the forefront in using diffraction-based techniques in scanning electron microscopy, including being a leader in the development of electron channeling contrast imaging (ECCI) and high resolution selected area channeling patterns (HR-SACP) for the characterization of crystal defect structures in bulk materials. His core research programs deal with the study of deformation and fracture initiation in structural metals, including titanium alloys, tantalum, and intermetallic compounds, while he also applies these technique to a variety of research topics, including carbon nanotubes, magnetic multilayers, and ceramic joining. He brings this experience to the classroom, teaching courses in electron microscopy, x-ray diffraction, physical metallurgy, and deformation and fracture mechanisms. He has published approximately 150 archival journal and proceedings papers. He currently sits on the editorial board of the *International Journal of Plasticity* and is a key reader for *Metallurgical and Materials Transactions*. He served as a member of the Committee on Technologies to Deter Currency Counterfeiting; the Board of Manufacturing and Engineering Design; and the National Research Council of the National Academies. He has been appointed as a guest professor at Harbin Institute of Technology, Harbin, PRC, as a visiting scientist a the Max-Plank-Institute für Eisenforschung, Dusseldorf, Germany, and as a visiting 1st Class Professor at the Université of Lorraine, Metz, France. He currently serves as vice-chairperson of the MSU Faculty Senate.

BRUCE E. DALE (PP. 14–15)

Bruce E. Dale is an MSU University Distinguished Professor within the Department of Chemical Engineering and Materials Science, a researcher in the Composite Materials and Structures Center, an MSU AgBioResearch scientist, and a participant in the Great Lakes Bioenergy Research Center. He also serves as editor-in-chief of *Biofuels, Bioproducts & Biorefining* (Biofpr). He received his bachelors (summa cum laude) and masters degrees in chemical engineering from the University of Arizona in Tucson and a PhD from Purdue University in 1979, under the direction of Dr. George T. Tsao, one of the early pioneers in biochemical engineering. Dr. Dale has spent his entire 30-plus-year career studying ways to turn biomass (plant leaves and stems, tree trunks and branches) into biofuels. He won the Charles D. Scott Award (1996) for contributions to the use of biotechnology to produce fuels and chemicals and the Sterling Hendricks Award (2007) for contributions to agriculture. He was named a Fellow of the American Institute of Chemical Engineers in 2011 and received the Award of Excellence of the Fuel Ethanol Workshop (also 2011). At number 14, he is the highest-ranked academic in the Top 100 People in Bioenergy (*Bioenergy Digest*), and was recently inducted into the American Institute for Medical and Biological Engineering (AIMBE) College of Fellows. He has published more than 250 journal papers and hold 42 U.S. and international patents. Research interests include biofuels, the relationship between energy and societal wealth, life cycle assessment, and the design of integrated agroecosystems for producing sustainable fuels, chemicals, food, and animal feed.

LAWRENCE T. DRZAL (PP. 16–17)

Lawrence T. Drzal is an MSU University Distinguished Professor within the Department of Chemical Engineering and Materials Science, and director of the Composite Materials and Structures Center. He conducts research on the synthesis, functionalization, processing, and manufacturing of carbon and glass fiber reinforced composite materials and graphene, nano-cellulose, and boron nitride nanomaterials. His current foci are on the combination of nanomaterials with fiber-reinforced composites to produce multifunctional composite materials and the investigation into the use of inexpensive graphene nanoplatelets for various applications. Research from Drzal's group has led to a commercially viable method for manufacturing graphene nanoplatelets, which have multiple desirable intrinsic properties that make them particularly attractive as additives to polymers and composites as well as for energy storage applications. Full advantage of these multifunctional nanomaterials requires not only a high level of dispersion but also novel processing methods to generate 2D and 3D microstructures within the polymers in which they are dispersed. Professor Drzal's group is investigating chemical, electrical, and flow methods to induce desirable structure of nanomaterials by themselves as well as within polymers to optimize their performance in structural and energy generation and storage applications. Professor Drzal and his students have published over 350 journal articles, been granted 35 patents, and spun off a company (XG Sciences) to manufacture graphene nanoplatelets. Professor Drzal has received numerous awards for his research and has been elected a Fellow in six national professional societies.

PHILIP EISENLOHR (PP. 18–19)

Philip Eisenlohr is an associate professor in the Department of Chemical Engineering and Materials Science. Prior to his present position he was leading a research group on Computational Mechanics of Polycrystals at the Max-Planck Institut für Eisenforschung GmbH (Düsseldorf, Germany) for seven years and held an appointment as a research and teaching assistant at the Universität Erlangen-Nürnberg, Germany, before that. He received both an MS (1999) and PhD (2004) from the Universität Erlangen-Nürnberg in materials science and engineering (with distinction). In 2001, he was the recipient of the young investigator award of the German Society of Materials Science (DGM). His particular field of interest is the computational prediction of advanced structural material performance by considering interactions of microstructure and plasticity in crystalline solids. He has published more than 60 papers in international peer-reviewed journals and contributed book chapters and one monograph in the general field of crystal plasticity.

MARTIN HAWLEY

Martin Hawley is a professor and chairman-emeritus of the Department of Chemical Engineering and Materials Science, Senior Associate to the Dean of Engineering, and director of the Composite Vehicles Research Center (CVRC). He directs research in areas of chemical kinetics, transport phenomena, and enzyme separations. Present research is concerned with chemicals from biomass; free radical production in microwave plasmas; electromagnetic coupling and measurements for materials processing; and basic reaction and transport studies in thick-section composites. Dr. Hawley consults for industry and government in areas of computer simulation, chemical reactor design, process design, and materials processing. Previously, he was co-director of the NSF-supported State of Michigan/Industry/University Cooperative Research Center on Low-Cost, High-Speed Polymer Composites Processing. He also recently served as director of the MSU Office of Sponsored Programs. Dr. Hawley holds six patents and has published more than 200 articles and books. He and his co-authors received the 2014 *Composites Part A* Most Highly Cited Paper Award, for having received the most citations in the preceding five years in the *Elsevier Journal of Composites Part A*. Dr. Hawley was named Chemical Engineer of the Year (1975 and 1976) by the Mid-Michigan Section of AIChE, and was recognized with an MSU Distinguished Faculty Award (1982). During his tenure as chair, the ChEMS department grew tremendously in size and stature: increasing its faculty by about 50 percent, nearly doubling the student body, and increasing research expenditures by a factor of five. Dr. Hawley holds both a BS (1961) and PhD (1964) in chemical engineering from Michigan State University, and has been a member of the faculty since 1964.

DAVID HODGE (PP. 20–21)

David Hodge is an associate professor in the Department of Chemical Engineering and Materials Science with a joint appointment in the Department of Biosystems and Agriculture Engineering, and a participant in the Great Lakes Bioenergy Research Center.. Dr. Hodge's research addresses the challenges associated with the conversion of plant-derived biomass to renewable fuels and chemicals with support from DOE, NSF, and USDA. He received a BS degree in Chemical Engineering from Auburn University with a specialization in pulp and paper engineering and obtained MS and PhD degrees in chemical engineering from Colorado State University. This was followed by work at the U.S. Department of Energy's National Renewable Energy Laboratory as post-doctoral researcher and a subsequent research faculty position at Luleå University of Technology in Sweden. He was a 2014 fellow of the MSU Academy for Global Engagement.

KRISHNAMURTHY JAYARAMAN (PP. 22–23)

Krishnamurthy Jayaraman is a professor in the Department of Chemical Engineering and Materials Science, and a researcher in the Composite Materials and Structures Center. Dr. Jayaraman's research group is developing processing strategies, flow models and design tools for shaping polymeric materials into products for various industry sectors: automotive, energy and building or construction. This research is applied to develop processing strategies for polymer composites, recycled polymers and polymer nanocomposites to make foam core panels, multilayer blown film, stronger light weight building materials and porous plastic sheets. Dr. Jayaraman's research interests and expertise are processing, rheology, and microstructure development in polymer materials. These include composites, polymer nanocomposites, foams and porous composite products, thermoplastic olefin blends, elastomers, thermoplastic foams and thermoplastic vulcanizate blends (TPV). Current research projects include nonlinear rheology of polyamide based TPVs for extrusion and film blowing, die-drawing of porous polymer membranes for battery separators, texture development in die-drawn expanded polypropylene-talc composites, high-performance additives with nanoparticles for masking film in paint ovens, and modeling of expanding foam flow due to reaction in heated mold cavities with distributed vents. He received both an MS (1973) and PhD (1975) in chemical engineering from Princeton University, in Princeton, NJ.

WEI LAI (PP. 24–25)

Wei Lai is an associate professor in the Department of Chemical Engineering and Materials Science. His research interests are focused on the advanced materials and electroanalytical methods for energy storage and conversion applications. Recent research efforts in his lab have centered on Solid-state Ionic Conductors (SIC) and Solid-state Mixed Ionic and Electronic Conductors (SMIEC) as battery electrolytes/electrodes and thermoelectric (TE) materials. He received his BS (1998) and MS (2001) in materials science from the University of Science and Technology of China, and his PhD in materials science from the California Institute of Technology (in 2007). Before joining MSU, he was a postdoctoral associate in the Department of Materials Science and Engineering at the Massachusetts Institute of Technology. Dr. Lai is a 2016 fellow of the MSU Academy for Global Engagement.

ANDRE LEE (PP. 26–27)

Andre Lee is an associate professor in the Department of Chemical Engineering and Materials Science, and a researcher in the Composite Materials and Structures Center. His research interests include viscoelastic and time-dependent properties of polymers and polymeric glasses, structure-property relationships of inorganic-organic hybrid polymers and nanocomposites, processing of hybrid nano-reinforced polymer, and nanostructured materials. He received both an MS in physics (1982) and PhD in physics/materials science (1987) from University of Illinois, Urbana. He worked at the National Institute of Standards and Technology (NIST) and the Lockheed Corporation prior to joining MSU in 1991.

ILSOON LEE (PP. 28–29)

Professor Ilsoon Lee is an associate professor in the Department of Chemical Engineering and Materials Science. His research interests include molecular level control over self-assembled bio-thin films and nanostructured films via novel non-lithographic approaches, molecular self-assembly, and layer-by-layer assembly. His expertise also includes the nanofabrication and characterization of nanomechanical wrinkle free films, anisotropic functional nanoparticles, and high-surface and high-selectivity bioelectronic interfaces for biosensors, biocatalytic reactors, and biofuel cells. He received an MS in chemical engineering (1995, Summa Cum Laude) from Seoul National University in South Korea, and a PhD in chemical engineering from the University of Delaware (2000), followed by postdoctoral research at the Massachusetts Institutes of Technology.

CARL T. LIRA (PP. 30–31)

Carl T. Lira is an associate professor in the Department of Chemical Engineering and Materials Science. He teaches thermodynamics at all levels, chemical kinetics, and material and energy balances. His research accomplishments include experimental measurements and modeling for liquid metals, supercritical fluids, adsorptive separations, and liquid-vapor, solid-liquid, and liquid-liquid phase equilibria. Dr. Lira specializes in the study of thermodynamic properties of bio-derived fuels and chemicals via experiments and molecular simulations, and he collaborates in the MSU Reactive Distillation Facility. He has been recognized with the Amoco Excellence in Teaching Award, and multiple presentations of the College of Engineering Withrow Teaching Excellence Award. He holds a BS from Kansas State University, and an MS (1984) and PhD (1986) from the University of Illinois, Champaign-Urbana, all in chemical engineering. He is co-author of the market-leading textbook *Introductory Chemical Engineering Thermodynamics*, and he is involved in educational research using lexical analysis to interpret student misconceptions in thermodynamics.

RICHARD R. LUNT (PP. 32–33)

Richard R. Lunt is the Johansen Crosby Endowed Associate Professor at Michigan State University in the Department of Chemical Engineering and Materials Science where his group focuses on understanding and exploiting excitonic photophysics and molecular crystal growth to develop unique thin-film optoelectronic devices. He earned his BS from the University of Delaware in 2004 and his PhD from Princeton University in 2010. He then worked as a post-doctoral researcher at MIT until 2011. His work has been featured in *Nature*, *The New York Times*, Huffington Post, CNN, CBS, and NBC News, among others, and his innovative research has earned him a number of prestigious awards including the NSF CAREER Award, the Camille and Henry Dreyfus Mentor Award, the DuPont Young Investigator Award, the APS Ovshinsky Award, and was named to the *Technology Reviews*' Top 35 Innovators Under 35. He is the inventor of over 15 patents, the majority of which have been licensed, and is a founder of Ubiquitous Energy Inc., which is commercializing a range of seamless light-harvesting technologies.

DENNIS MILLER (PP. 34–35)

Dennis Miller is a professor in the Department of Chemical Engineering and Materials Science. His research group focuses on the development of chemical pathways, catalysts, and processes to produce chemicals and biofuels from renewable biomass resources. Research projects involve both the development of new catalysts and reactor designs to carry out conversion of feedstocks to desired products, and the separation and purification of products from the reaction mixtures. Major efforts in current work are in reactive separations, where the chemical reaction and purification take place in a single process unit, and in upgrading low-cost intermediates from biomass such as ethanol and furan-based compounds to higher-profit products. Twenty U.S. patents along with numerous publications have come out of this work, and several technologies have been licensed for commercial development. Dr. Miller has been recognized numerous times with the College of Engineering Withrow Teaching Excellence Award, and received the MSU Distinguished Faculty Award in 2013. He holds both an MS (1978) and PhD (1982) in chemical engineering from the University of Florida, Gainesville.

DONALD MORELLI (PP. 36–37)

Donald Morelli is a professor of materials science, interim chair of the Department of Chemical Engineering and Materials Science, and director of the Center for Revolutionary Materials for Solid State Energy Conversion (U.S. DOE Energy Frontier Research Center). Prior to joining MSU in 2007, he spent 21 years in industry, first at General Motors Research Laboratories as a senior research scientist, before moving to Delphi Corporation Research Labs in 1999, where he was staff research scientist and group leader of the nanomaterials group. Dr. Morelli received two GM Campbell Awards (1992 and 1997) for fundamental scientific research, the International Thermal Conductivity Conferences Fellowship Award (1993), and the Delphi Scientific Excellence Award (2004). He has been elected Fellow of the American Physical Society (2005) and was inducted into the Delphi Corporation Innovation Hall of Fame (2006). He currently serves as president of the International Thermoelectric Society. He has published more than 150 scientific papers, coauthored four book chapters, and received 23 U.S. patents. His research has spanned a variety of topics, including: semimetals, conducting polymers, high temperature superconductors, wide and narrow band gap semiconductors, high thermal conductivity crystals, thermoelectric materials, and magnetism. Dr. Morelli's research group at MSU continues to emphasize new semiconductors for thermoelectric energy conversion, as well as materials for thermal management. Dr. Morelli holds both BS (1981) and PhD (1985) degrees in physics from the University of Michigan.

RAMANI NARAYAN (PP. 38–39)

Ramani Narayan is an MSU University Distinguished Professor within the Department of Chemical Engineering and Materials Science, and a researcher in the Composite Materials and Structures Center. His research encompasses design and engineering of sustainable, biobased products, biodegradable plastics and polymers, biofiber reinforced composites, reactive extrusion polymerization and processing, studies in plastic end-of-life options like biodegradation and composting. He has 200 refereed publications, and 29 issued patents in bioplastics, and is a successful entrepreneur, having commercialized several biobased and biodegradable product technologies. His work has been recognized by numerous industry and academic organizations, including the first lifetime achievement award from the BioEnvironmental Polymer Society (BEPS), the (Michigan) Governor's University Award for commercialization excellence, the Green Chemistry

Governor's Award, and DuPont's Packaging Award as part of the Coca Cola bottle team. He is an elected Fellow of the U.S. National Academy of Inventors (2015) and the ASTM, in addition to numerous other recognitions for his contributions to ASTM. He has been a recipient of the MSU Distinguished Faculty Award (2006) and the College of Engineering Withrow Distinguished Scholar Award (2005), and held the Fulbright Distinguished Lectureship Chair in Science and Technology Management and Commercialization (University of Lisbon; Portugal). Dr. Narayan is scientific chair of the Biodegradable Products Institute (BPI); technical advisor to the WWF BioPlastic Feedstock Alliance, and convener/technical expert on ISO, & ASTM Standards writing committees. He holds both an MS (1969) and PhD (1975) from Bombay University, in organic chemistry.

JASON D. NICHOLAS (PP. 40–41)

Jason Nicholas is an assistant professor in the Department of Chemical Engineering and Materials Science. His research interests include solid state ionics, nano-composite electrode fabrication, and the use of strain to engineer the properties of electrochemically active devices. He obtained a Master's Degree in materials science from the University of Illinois at Urbana-Champaign in 2003, a PhD in materials science from the University of California, Berkeley in 2007. After completing a post-doc at Northwestern University in 2009, he joined the faculty at Michigan State University in 2010. He was the recipient of a 2013 Withrow Teaching Award and a 2013 National Science Foundation CAREER Award. He is active in advocating the benefits of solid oxide fuel and electrolysis cells, and organized the 2013 NSF SOFC Promise, Progress, and Priorities Workshop (https://www.sofcwg.org). Updates on his research can be found at https://www.egr.msu.edu/nicholasgroup.

ROBERT OFOLI (PP. 42–43)

Robert Ofoli is an associate professor in the Department of Chemical Engineering and Materials Science. His research addresses the need for sustainable production of energy and materials. His primary interest is in the synthesis, characterization, assessment, and optimization of nanoscale catalysts and complexes that efficiently achieve the required transformations. Dr. Ofoli's team focuses on four technological goals: reaction specificity; high reactivity under moderate reaction conditions; catalyst robustness and recyclability; and development of generic protocols to enable easy adaptation to other feedstock and products. The team's general approach is to integrate rational catalyst design and synthesis, characterization and assessment, and modeling and simulation to understand structure-function relationships. Dr. Ofoli is currently focusing on two areas of significant scientific and societal interest: biomimetic water oxidation to produce hydrogen and organic materials, and transformation of renewable materials to high-density liquid fuels capable of replacing those traditionally obtained from crude oil. Dr. Ofoli holds two PhD degrees: in agricultural engineering from MSU (1984) and chemical engineering from Carnegie Mellon University (1994). He has been recognized twice with the College of Engineering Withrow Teaching Excellence Award, and received the Gary Leach Award from the American Institute of Chemical Engineers in 2007.

CHARLES PETTY (PP. 44–45)

Charles Petty is a professor in the Department of Chemical Engineering and Materials Science, and a researcher in the Composite Materials and Structures Center. His Research interests include: hydrodynamic and reactor stability theory; solid-fluid separations; and turbulent transport phenomena. Turbulent flows occur ubiquitously with numerous examples in engineering, atmospheric science, oceanography, astrophysics, biology, and environmental science. Dr. Petty is currently developing improved models for turbulence that will have a direct impact on the current use of advanced computational fluid dynamic methods for process design, process diagnostics, and process safety assessments by engineers and others. The results will support the discovery of new flow phenomena in disciplines that depend on accurate predictions of the mean velocity field and the mean pressure field. The goal is to develop a new class of low-order turbulent closure models that account for the transport of momentum, energy, and chemical constituents within single-phase (and multiphase) rotating and non-rotating turbulent flows. He holds both a BS (1966) and PhD (1970) in chemical engineering from the University of Florida, Gainesville.

YUE QI (PP. 46–47)

Dr. Yue Qi is an associate professor in the Chemical Engineering and Materials Science Department. She received her PhD in materials science from the California Institute of Technology in 2001. She was a co-recipient of the 1999 Feynman Prize in Nanotechnology for Theoretical Work during her doctoral studies. She worked for 12 years working at the Chemical Sciences and Materials Systems Lab, General Motors R&D Center, Warren, MI. At GM, she won three GM Campbell awards for outstanding research on various topics and the TMS Young Leader Professional Development Award. Her recent research interest is integrating material failure model with battery life prediction. She has published more than 100 peer-reviewed journal papers with more than 3000 citations. Recently, she has been awarded a 2017 Brimacombe Medal from The Minerals, Metals and Materials Society for significant contributions in multidisciplinary computational materials science.

■ S. PATRICK WALTON (PP. 48–49)

S. Patrick Walton is an associate professor in the Department of Chemical Engineering and Materials Science, and director of the College of Engineering CoRe Experience. One achievable goal of the 21st century is "personalized medicine," the design of diagnostics and therapeutics specifically for a single patient. The Applied Biomolecular Engineering Laboratory (ABEL), led by Dr. Walton, is currently working on development of both novel therapeutics and diagnostics, specifically on technologies that rely on nucleic acids (i.e., DNA and RNA). Areas of investigation include designing nucleic acid–based therapeutics based on understanding their mechanism of action, and developing diagnostics to measure protein levels in parallel. Recent foci have been a new class of therapeutics, short, interfering RNAs, with the goal of developing guidelines for designing these molecules. Additionally, Dr. Walton is developing a technique for parallel measurements of transcription factors, proteins that help the cell respond to stimuli, using a solution-phase magnetic bead-based approach. He holds both an MS in chemical engineering practice (2000) and ScD (2002) in chemical engineering from the Massachusetts Institute of Technology. He has been recognized as a member of Who's Who in Engineering Education (2005), and received the MSU Teacher-Scholar Award in 2010.

■ TIM WHITEHEAD (PP. 50–51)

Tim Whitehead is an assistant professor in the Department of Chemical Engineering and Materials Science, with a joint appointment in the Department of Biosystems and Agricultural Engineering. His laboratory is geared toward converting biomass into next-generation fuels and chemicals, and also developing proteins for a wide range of treatment areas. For proteins, imparting novel and specific functions is a difficult problem because protein structures are only marginally stable, protein structure-function relationships are not well understood, and many targeted small molecule substrates differ by as little as a single hydroxyl group or a methyl bond. Dr. Whitehead's research group is working to solve the problem of engineering proteins. They use and develop computational techniques to design proteins for new functions, have pioneered experimental approaches to comprehensively assess the effect of a protein's sequence on its desired function, and have imparted evolutionary and computational ideas to formulate efficient routes to optimize protein function. Dr. Whitehead is interested in optimizing proteins for diverse applications like vaccine design and creating the next generation of biofuels. He received a BE in chemical engineering from Vanderbilt University in 2001, and a PhD in chemical engineering from the University of California–Berkeley in 2008. He was the recipient of a prestigious CAREER award from the National Science Foundation in 2013, and served as a fellow of the MSU Academy for Global Engagement in 2015.

■ R. MARK WORDEN (PP. 52–53)

Robert Mark Worden is a professor in the Department of Chemical Engineering and Materials Science, an MSU AgBioResearch scientist. An expert in biomedicine, Dr. Worden's research involves the application of engineering principles to biological systems. His lab has special expertise in the use of proteins as nanomachines, and in the production of high-value products utilizing enzymes and biological cells. Since joining MSU in 1986, Dr. Worden has conducted research and developed multidisciplinary educational programs in the areas of bioprocess engineering, nanobiotechnology, and bioelectronics. He has been recognized with the College of Engineering Withrow Teaching Excellence Award (2003–2004), and was recently inducted into MSU's inaugural chapter of the National Academy of Inventors. He holds a BS in chemistry and cell biology, and MS (1982) and PhD (1986) degrees in chemical engineering, all from the University of Tennessee.

■ ALEXANDRA ZEVALKINK (PP. 54–55)

Alexandra Zevalkink is an assistant professor in the Department of Chemical Engineering and Materials Science. Her research leverages crystal growth and high temperature characterization techniques to study the relationship between atomic structure and bonding and the electronic and thermal properties of functional inorganic materials. Recent efforts have focused on optical floating zone growth of single crystals and measurements of the high-temperature sound velocity and lattice expansion in materials used for thermoelectric energy conversion. Dr. Zevalkink received her BS from Michigan Technological University in 2008 and her PhD from the California Institute of Technology in 2014. After completing her PhD, she pursued postdoctoral research at the Jet Propulsion Laboratory in Pasadena, CA and at the Max Planck Institute for Chemical Physics of Solids in Dresden, Germany.

FACULTY RESEARCH

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RESEARCH INTERESTS

Value-added products from agricultural and forest raw materials

GROUP MEMBERS

Jacob Rochte, Nicole Shriner

CURRENT RESEARCH

Our group's activities are aimed at the creation of value-added products utilizing raw materials obtained from agricultural and forest raw materials. In particular, we utilize fermentation processes to develop integrated production for foods, beverages, biochemicals, and biofuels.

Beverage Technology. The artisan distilling industry in Michigan is poised to undergo significant expansion in the next few years resulting in positive economic impact for the state. Challenges for the entrepreneurs entering this business are access to technological expertise and facilities to develop and market products. An additional complication of the distilled spirits industry lies in the regulations governing it. Unlike beer and wine, there is no minimum amount of spirits that can be produced without Federal and State licenses. Furthermore, it is required to have constructed an operational distillery in order to apply for a Federal license. These regulations place the potential new producer in the position that in order to attract investment it is necessary to produce products and show their market value, but to do so, it is necessary to have the investment in a plant to get a license. We work to break this cycle by assisting new entrepreneurs in development and marketing of their spirits in order to attract the required investment for construction of their own facility.

Upgrading forest byproducts. Xylose derived from hemicellulose is a low-cost source of substrate for butyric acid fermentation given that extraction could be integrated into current industrial pulp and paper processes yielding hemicellulosic sugars for the fermentation while retaining the properties of the cellulose fraction to be used in the subsequent pulp production. One of the main issues concerning such an integration is that hydrolysis of hardwood hemicellulose releases not only xylose but also acetic acid (up to 40 g/L), a microbial inhibitor. To achieve biologically conversion of xylose to butyric acid, the inhibiting acetic acid must either be removed from the extraction broth or the fermentation strain adapted to tolerate such high levels. This study focuses on the impact of high levels of acetic acid on *C. tyrobutyricum* fermentation growth kinetics and product yields in order to establish a process with extracted xylose as a substrate without requiring the removal of the toxic acetic acid from the broth.

RECENT PUBLICATIONS

N. Bonturi, L. Matsakas, R. Nilsson, P. Christakopoulos, E.A. Miranda, K.A. Berglund, U. Rova. "Single cell oil producing yeasts *Lipomyces starkeyi* and *Rhodosporidium toruloides*: selection of extraction strategies and biodiesel properties prediction," *Bioenergy and Biofuel,* May 28, 2015.

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H. Alizadeh, K.A. Berglund. "Effects of airport runway deicers on standard test materials: potassium succinate vs. potassium salts of acetic and formic acids," *IJEART*, vol. 3, no. 4 (Aug.–Sept., 2015).

C. Johansson, K.A. Berglund. "Oxydehydrogenation of succinic acid to maleic acid and fumaric acid," *IJEART*, vol. 3, no. 4 (Aug.–Sept., 2015).

C. Johansson, K.A. Berglund. "Oxydehydrogenation of succimide to maleimide," *IJEART*, vol. 3, no. 4 (Aug.–Sept., 2015).

T. Petrik, K.A. Berglund. "The effects of different salts/acids on the vapor-liquid equilibrium of the binary system of water/ethanol," *IJEART*, vol. 3, no. 4 (Aug.–Sept., 2015).

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RESEARCH INTERESTS

Grain boundaries, crystallographic texture, crystal plasticity, microstructure evolution, damage nucleation

LAB(S)/GROUP(S)

Solder research group, Niobium research group, Titanium research group

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SPECIAL EQUIPMENT AVAILABLE

Orientation imaging microscopy, *in situ* deformation stage in SEM

GROUP MEMBERS

Chen Zhang, Harsha Phukan, Yang Su, Bret Dunlap, Jason Zhou, Aboozar Mapar, Di Kang, Mingmin Wang

PATENTS

"Composite solder production involves combining solder with the components of an intermetallic phase, heating the formed mixture, and rapidly cooling the formed non-solid mixture," T.R. Bieler, K.N. Subramanian, S. Choi. (Application filed 6/98, granted 6/17/2004, 8/10/2010).

"Apparatus for the preparation of metal matrix fiber composites," T.R. Bieler, L.T. Drzal, H. Wang, V.R. Yallapragada. US patent 5,891,249 (4/6/1999).

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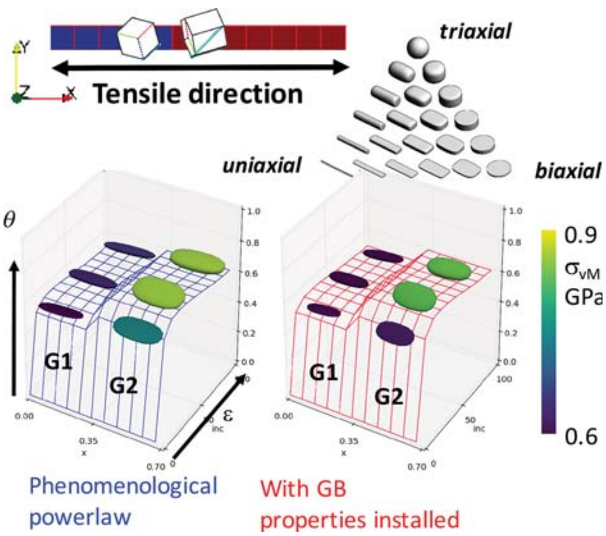

FIGURE 1. An accurate model of a 3D microstructure is constructed using a surface OIM scan and 13 DAXM scans.

CURRENT RESEARCH

Orientation Imaging Microscopy™ (OIM, aka EBSP mapping) is used to quantitatively examine the relationships between microstructure and localized deformation processes that ultimately control heterogeneous deformation, recovery and recrystallization mechanisms, and damage nucleation. Combined with other experimental and analytical tools, such as 3D x-ray diffraction, new insights on formability and damage nucleation mechanisms are found. This will enable development of optimal material processing strategies to gain more predictable and reliable properties. Three examples follow.

Damage nucleation in titanium and titanium alloys. Figure 1 shows computational deformation of a bicrystal that is oriented to enable slip transfer from a prism slip system (blue grain) that is perfectly aligned with a pyramidal slip system (red grain). While uniaxial tension is applied to the bicrystal, the restrictions of the anisotropic slip systems causes the stress state to deviate significantly from uniaxial tension. The left grain sees a stress state closer to uniaxial tesion and the right crystal is closer to biaxial tension. Normal crystal plasticity models allow slip transfer across grain boundaries by all slip systems. When slip is restricted on all except the one that is well-aligned, the magnitude of the stress is actually reduced (color scale on the right) and the shape of the stress tensor changes (glyphs). This provides evidence that more physically realistic deformation at grain boundaries can be installed into larger scale simulations.

Microstructural evolution during thermo-mechanical cycling in lead-free solder joints. Accelerated thermal cycling is often done on prototype electronic systems to identify weak links. This causes significant microstructural evolution in solder joints, which leads to cracking and eventual failure. The failure mechanisms were identified using OIM and DAXM measurements illustrated in Figure 2. Clockwise from the top, two cross sections of thermally cycled solder joints show that they originally solidified as single crystals, but after thermal cycling recrystallization took place near the interface with the package on top. The 'red' oriented joint is examined in greater detail, showing the developing crack. The region surrounding the crack has various recrystallized grain orientations (different colors), and surrounding red orientations are separated by low-angle grain boundaries (LAGB). The gold area in the local average misorientation (LAM) map shows higher degree of crystal perfection in recrystallized grains. A subsurface DAXM scan shows internal strains built up along the LAGBs, which attracts the migration of recrystallized grain boundaries. Thus the mechanism for crack growth is identified: (1) Anisotropic thermal expansion of Sn causes different stress states in every joint, LAGB develop within crystals by a continuous

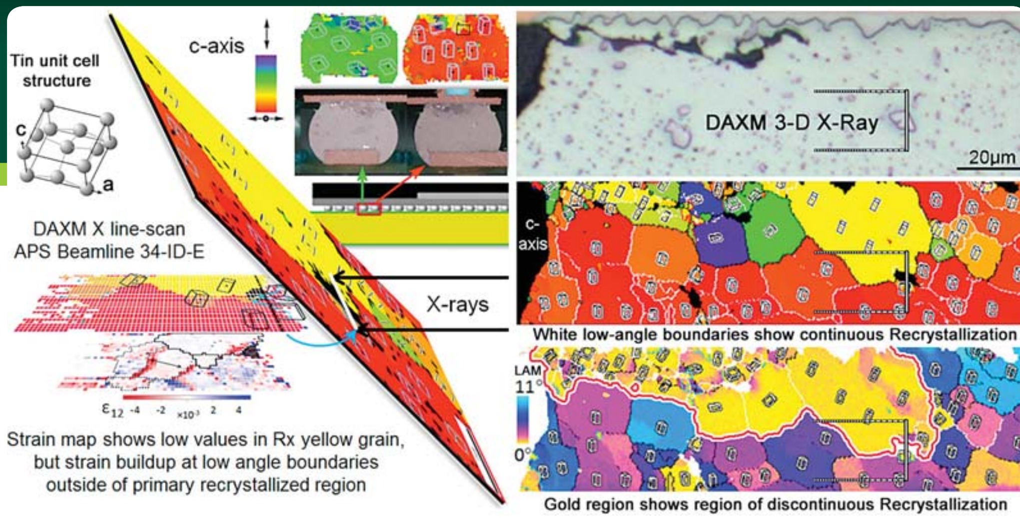

FIGURE 2. The mechanism of crack nucleation and growth was identified using OIM and DAXM.

recrystallization process, (2) Primary (discontinuous) recrystallization (random orientations) consume LAGB material, and (3) Anisotropic thermal expansion mismatch causes grain boundary sliding and voids in high-angle recrystallized grain boundaries that link up along boundaries and propagate the crack.

Characterization and modeling of deformation of defects in high purity Nb for particle accelerators. High purity Nb is used for radio frequency superconducting particle accelerator cavities (the structures that accelerate particles), but the fundamental physics of deformation and surface modification processes (which includes strong acid etching) and microstructure evolution are not well understood. Figure 3 illustrates how preferential magnetic flux penetration (red arrow) occurs along low angle grain boundaries, and may result from hydride precipitates that form during cooling. Hydrides leave scars when they dissolve upon reheating to room temperature. The hydride scars are misoriented by as much as 10° from the surrounding material, indicating that significant local straining occurred, leaving significant dislocations behind. Hydrogen is attracted to defects, so hydrides are markers of where dislocations are found. The relationship between dislocations, low-angle and high-angle boundaries is being examined to determine how their presence can be minimized by the time the cavity is formed.

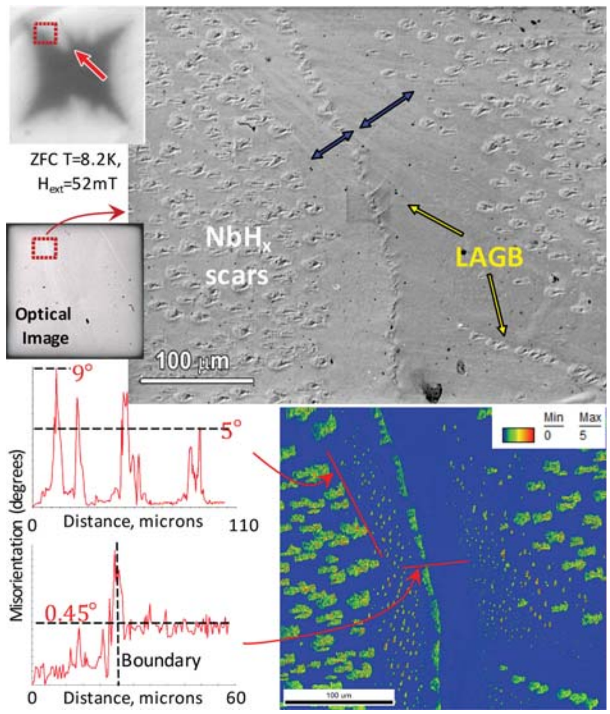

FIGURE 3. Upon cooling Nb to about 8K, magneto optical imaging reveals preferential flux penetration sites (red arrow, upper left image), which is correlated with low angle boundaries. Niobium hydrides form on the surface, and dissolve upon heating, but they leave scars revealed in an orientation map. It is unknown how they affect magnetic flux penetration.

RECENT PUBLICATIONS

C. Zhang, H. Li, P. Eisenlohr, W. Liu, C.J. Boehlert, M.A. Crimp, T.R. Bieler. "Effect of realistic 3D microstructure in crystal plasticity finite element analysis of polycrystalline Ti-5Al-2.5Sn," *International Journal of Plasticity* 69, 21–35, (2015).

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T.-K. Lee, T.R. Bieler, C.-U. Kim, H. Ma. *Fundamentals of Lead-Free Solder Interconnect Technology: From Microstructure to Reliability*, Springer, New York, 2015, 253 pp.

P. Darbandi, T.-K. Lee, T.R. Bieler, F. Pourboghrat. "Crystal plasticity finite element study of deformation behavior in commonly observed microstructures in lead free solder joints," *Computational Materials Science* 85, 236–243, (2014).

T.R. Bieler, D. Kang, D.C. Baars, S. Chandrasekaran, A. Mapar, G. Ciovati, N.T. Wright, F. Pourboghrat, J.E. Murphy, C.C. Compton G.R. Myneni. "Deformation mechanisms, defects, heat treatment, and thermal conductivity in large grain niobium," *Science and Technology of Ingot Niobium for Superconducting Radio Frequency Applications*, AIP Conf. Proc. 1687, 020002, 18 pp., 2015.

D. Kang, T.R. Bieler, C. Compton, "Effects of processing history on the evolution of surface damage layer and dislocation substructure in large grain niobium cavities," *PRST-AB* 18, 123501 (2015) (doi: 10.1103/PhysRevSTAB.18.123501).

Carl Boehlert

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RESEARCH INTERESTS
Physical metallurgy

LAB LOCATION
B338 Engineering Bldg.

WEBSITE
http://www.egr.msu.edu/~boehlert/group

SPECIAL EQUIPMENT AVAILABLE
Thermomechanical testing machine

GROUP MEMBERS
PHD STUDENTS: Uchechi Okeke, Aida Amroussia, Vahid Khademi, David Hernandez Escobar, JoAnn Ballor

RECENT ACHIEVEMENTS
NSF DMR MMN

CURRENT RESEARCH
The research group of Professor Carl Boehlert is concentrating on understanding the deformation behavior of hexagonal close packed metals, in particular titanium and magnesium alloys, under extreme environments. The environments include a combination of both elevated temperatures and irradiation, and a variety of loading conditions are being used to mimic component use in commercial applications. *In situ* testing methods have been developed which allow for characterizing the surface deformation behavior during deformation in order to understand the deformation evolution. The work is being sponsored by the NSF and the DOE and a Michigan State University Strategic Partnerships Grant. More recently, Boehlert's group is working on understanding severe plastic deformation processing effects on nanostructured zinc magnesium alloys targeted for biomedical implant applications. Below is a brief description of a recent research project performed in Boehlert's group.

In situ electron backscattered diffraction (EBSD) heating experiments are typically performed to enable the understanding of phase transformations and/or recrystallization behavior as a function of temperature and time. Such experiments have been used to study the microstructural evolution and recrystallization in aluminum, copper, titanium, and steel. Similar studies help explain the microstructural evolution in wrought magnesium (Mg) alloys, in which the crystallographic texture has significant influence on the anisotropy in mechanical properties.

Rare earth (RE) containing Mg alloys form weaker textures during wrought processing (and subsequent annealing) than conventional Mg alloys. However, the underlying mechanisms responsible for this texture development in Mg alloys during annealing are not well understood. Therefore, an *in situ* annealing technique combined with EBSD was developed in order to characterize the microstructural evolution as a function of temperature in a RE-containing Mg alloy, Mg-2Zn-0.2Ce (wt%) (ZE20).

The ZE20 alloy studied features a measured composition of Mg-1.9Zn-0.2Ce (wt%). Samples were mechanically polished using silicon carbide grinding papers. To further improve sample surface quality for EBSD, specimens were electropolished using a solution of 30% nitric acid and 70% methanol as an electrolyte and a Struers TenuPol-5 double jet system. Figure 1 shows the experimental setup used for the *in situ* heating experiments.

An EBSD orientation map of a ~100 × 100 μm microstructural patch was initially acquired at 298 K using EDAX TSL OIM Data Collection v6.1 software. The specimen was heated to a target temperature (423 K) and held for ~15 minutes to stabilize the temperature. An EBSD map of the same microstructural patch was then acquired while the sample was held at 423 K. The heating and subsequent EBSD mapping cycle was then continued up to a desired temperature. EBSD maps were acquired at 298 K, 423 K, and at 473 to 598 K with 25° increments.

Figure 2 shows the EBSD inverse pole figure (IPF) map, corresponding texture in the form of {0001} pole figures (along the normal direction of the sample), and the grain orientation spread map of the same microstructural patch depicting the microstructure evolution as a function of annealing temperature. During the heating process, new grains appeared during the heating step from 473 to 498 K (Fig. 2). As expected, with new grain formation, the texture intensity in the

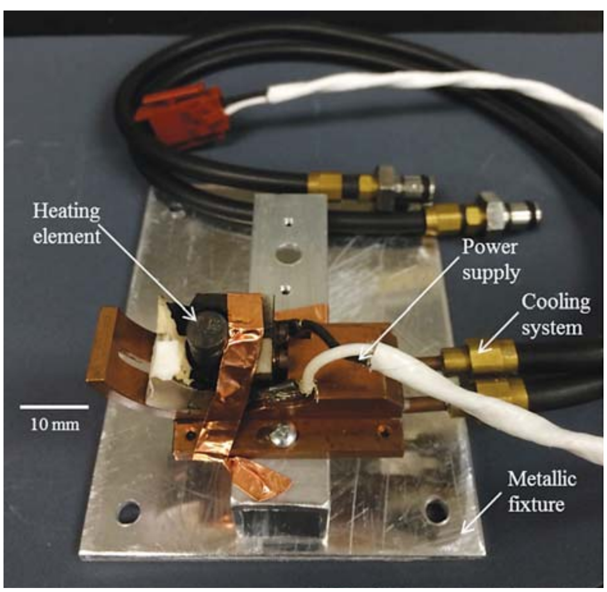

FIGURE 1. Heating stage used for *in situ* heating experiments. The sample (not shown) was placed directly on top of the heating element during the experiments.

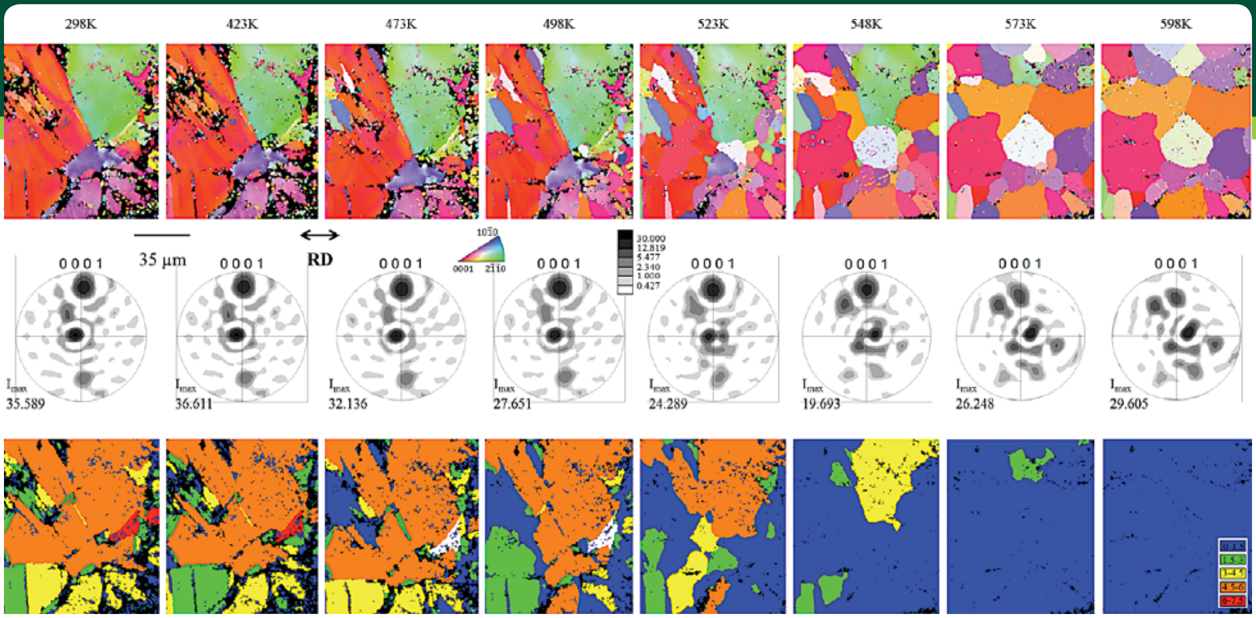

FIGURE 2. EBSD IPF map (*top*), corresponding texture in the form of {0001} pole figures (along the normal direction of the sample) (*middle*), and grain orientation spread map (*bottom*) of the same microstructural patch depicting the evolution of microstructure in rolled ZE20 as a function of temperature. Black regions in the maps are un-indexed points. Imax is the maximum intensity values observed in the pole figures.

microstructural patches decreased (Fig. 2). However, texture intensity increased slightly during the final heating steps, which included temperatures above 548 K. This was expected to be due to grain growth, where therefore fewer grains were present in the given microstructural patch analyzed. The orientation spread within the grains was less than 1.5° in the area analyzed after the 548–573 K heating step, suggesting that the grains were relatively free of strain accumulated during rolling. At 573 K, a completely recrystallized microstructure was observed.

In summary, recrystallization started at ~473 K. A completely recrystallized microstructure with relatively equiaxed and strain-free grains was observed at 548-573 K, and grain growth was observed thereafter. The characterization methodology developed in this work sets the stage for future experiments to understand and control the recrystallization behavior of commercial alloys. Future work is targeted at employing this technique to understand the effect of RE content on the recrystallization behavior of Mg alloys.

RECENT PUBLICATIONS

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A. Chakkedath, C.J. Boehlert, D. Escobar-Hernandez, J. Bohlen, S. Yi, and D. Letzig, “In-situ EBSD technique characterizes microstructural evolution of magnesium alloy,” *Advanced Materials and Processes*, June (2016) Vol. 174 No. 6, pp. 19–21.

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H. Wang, C.J. Boehlert, Q. Wang, D. Yin, and W. Ding, “In-situ analysis of the tensile deformation modes and anisotropy of extruded Mg-10Gd-3Y-0.5Zr (wt.%) at elevated temperatures,” *International Journal of Plasticity*, Vol. 84 (2016) 255–276. (http://dx.doi.ord/10.1016/j.ijplas.2016.06.001)

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V. Khademi, C.J. Boehlert, and M. Ikeda, “The tensile deformation behavior of beta titanium alloys at elevated temperatures,” *Proceedings of the Twenty-Fourth International Symposium on Processing and Fabrication of Advanced Materials* (PFAM XXIV), eds. M. Ikeda, T. Haruna, M. Niinomi, and T.S. Srivatsan, organized by Kansai University (Osaka, Japan), 2016, pp. I–X.

H. Wang, C.J. Boehlert, Q.D. Wang, D.D. Yin, and W.J. Ding, ”Analysis of slip activity and deformation modes in tension and tension-creep tests of cast Mg-10Gd-3Y-0.5Zr (wt pct) at elevated temperatures using in-situ SEM experiments,” *Metallurgical and Materials Transactions A*, Vol. 47 issue 5 (2016) 2421–2443. (doi: 10.1007/s11661-016-3383-0)

H. Wang, Q.D. Wang, C.J. Boehlert, J. Yang, D.D. Yin, J. Yuan, and W.J. Ding, “The impression creep behavior and microstructural evolution of cast and cast-then-extruded Mg-10Gd-3Y-0.5Zr (wt.%),” *Materials Science and Engineering A*, Vol. 649 (2015) 313–324.

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RESEARCH INTERESTS

Electrochemistry and electrocatalysis, from theory to experiment

LAB

Electrochemical Energy Lab (3250 Engineering Bldg.)

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GROUP MEMBERS

STUDENTS AND/OR COLLABORATING FACULTY: Yuanchao Liu, Kanchan Chavan, Alex Mirabal, Jacob Anibal, Fiona Nanney

CURRENT RESEARCH

Our research addresses engineering and materials issues in fuel cells, particularly mass transport within fuel cell electrodes. We focus on non-precious metal catalysts based on redox enzymes and transition metals, which have lower costs compared to precious metals, but are challenging in terms of overall activity and stability and often are implemented at high loadings that lead to transport limitations. Below are brief descriptions of current projects.

Metal nitrogen carbon (MNC) oxygen reduction catalysts for automotive fuel cells. We are developing a new process for inexpensive Metal-Nitrogen-Carbon (MNC) catalysts for oxygen reduction cathodes. High-pressure pyrolysis yields active MNC

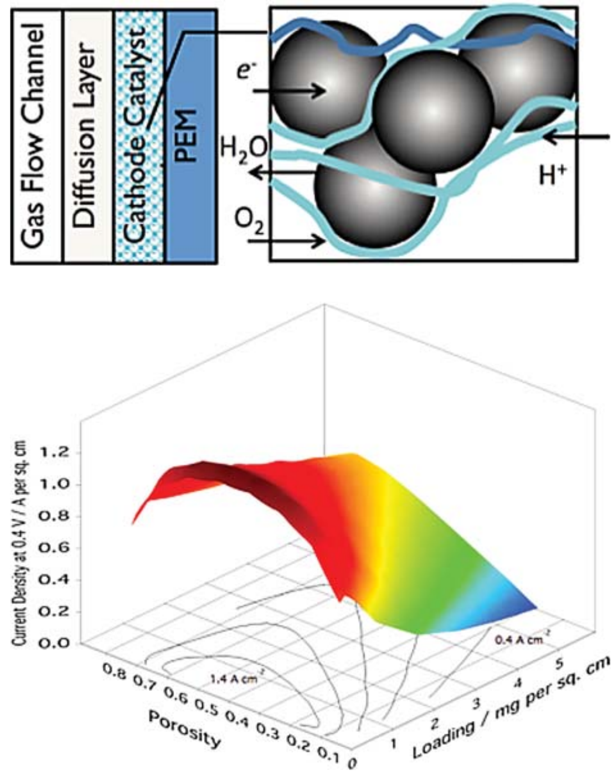
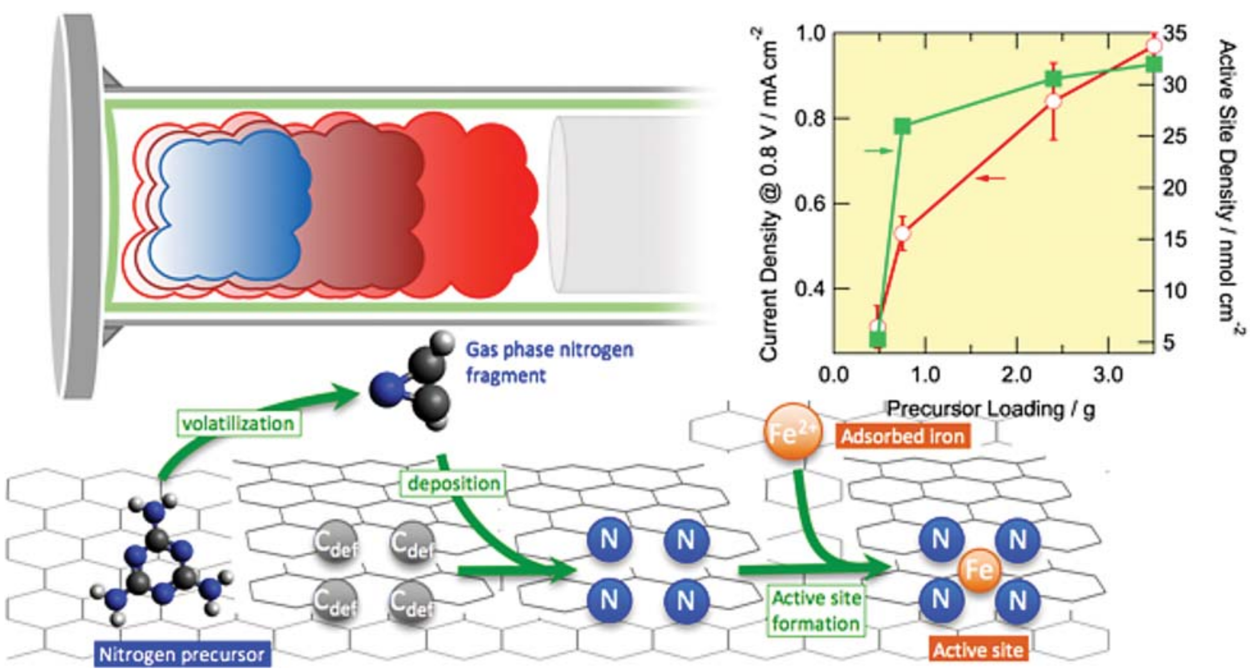


FIGURE 2. Cathode model schematic and optimization results. Maximum performance at low voltage (high current density) is achieved at low catalyst loading.

FIGURE 1. High-pressure pyrolysis process for non-precious metal catalyst production. Retention of volatile intermediates leads to increased Nitrogen activity and site density.



catalysts from transition metal (iron or cobalt) and nitrogen precursors (pyridine, melamine) combined with high surface area carbon materials in a closed, constant volume reactor (Figure 1). Activity approaches that of precious-metal platinum in acid and alkaline electrolytes.

We study the performance of these catalysts within a fuel cell cathode layer using numerical modeling techniques. Using our model, we have identified opportunities to optimize the design for improved performance, including reduced catalyst layer thickness and increased hydrophobicity of catalyst layer materials (Figure 2).

Bio-inspired design of adaptive catalysis cascades. As new catalytic systems are created for the production of advanced materials, energy conversion and harvesting, and human/machine interfaces, it is clear that natural pathways provide essential clues that will inspire novel designs. In this collaboration we are developing integrated catalytic cascades created from different catalytic modalities to optimize selectivity, electron transfer, diffusion, and overall pathway flux. The contribution of our laboratory is to quantitatively model the coupling of these novel catalytic steps and to study the transport of intermediates between steps (Figure 3).

Electrospun nanofibers for transition metal electrocatalalysis and bioelectrocatalysis. Introduction of non-precious electrocatalysts to electrochemical processes is plagued by poor transport properties owing to the large catalyst loading of relatively low-activity catalysts. We are to developing two classes of electrocatalysts based on electrospun carbon nanofibers. Electrospinning is a well-established, industrial-scale process producing carbon fibers with diameters ranging from 100 nm to over 1 micron and can be engineered with a range of structural, morphological, and surface properties for engineering and control of advanced porous electrodes (Figure 4). We implement these materials in two ways: (a) as precursor materials for preparation of metal-nitrogen-carbon (MNC) electrocatalysts for oxygen reduction, and (b) as support materials for preparation of enzymatic bioelectrodes. MNC electrocatalysts have applicability to low-temperature fuel cells for transportation and portable power. Bioelectrodes may be applied to biosensor, chemical conversion, and small-scale portable power environments.

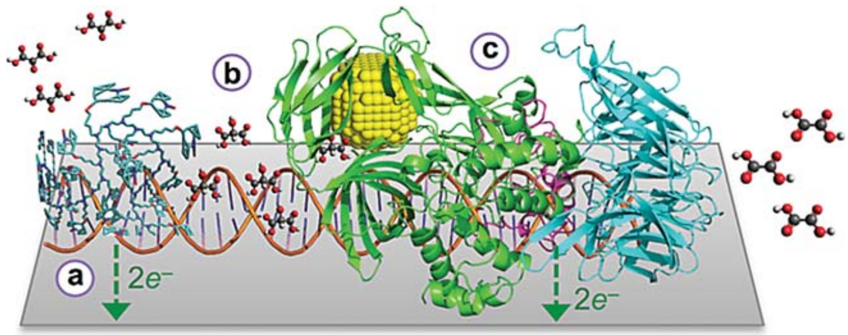


FIGURE 3. (A) Tartronic acid oxidation to mesoxalic acid at TEMPO catalyst; (B) facilitated transport of mesoxalic acid along DNA; (C) oxidation of mesoxalic acid to oxalic acid via catalysis by PtRu nanoparticle – AldDH adduct.

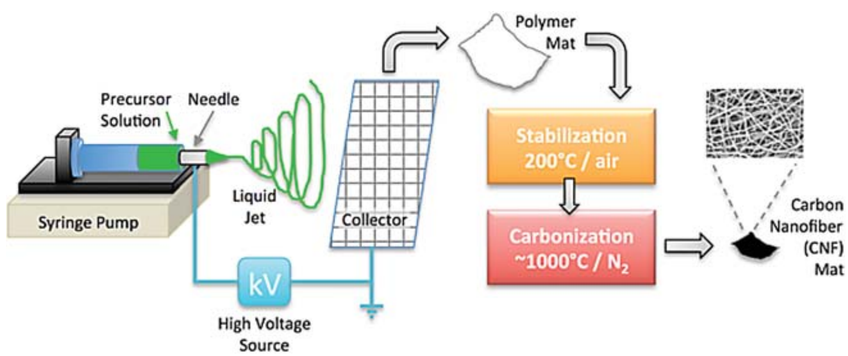


FIGURE 4. A basic experimental setup for electrospinning, followed by thermal treatment to produce carbon nanofiber (CNF) mats.

RECENT PUBLICATIONS

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D. Chakraborty, E. McClellan, R. Hasselbeck, S.C. Barton. "Characterization of enzyme-redox hydrogel thin-film electrodes for improved utilization," *J. Electrochem. Soc.*, 161, H3076–H3082 (2014). (doi:10.1149/2.0121413jes)

N.D. Leonard, S.C. Barton. "Analysis of adsorption effects on a metal-nitrogen-carbon catalyst using a rotating ring-disk study," *J. Electrochem. Soc.*, 161, H3100–H3105 (2014). (doi:10.1149/2.0161413jes)

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RESEARCH INTERESTS

Disease mechanisms, system biology, drug delivery, and tissue engineering

WEBSITES

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LABS

Cellular & Molecular Laboratory
Integrative Systems and Computational Biology Laboratory

GROUP MEMBERS

Ryan Thompson, Daniel Vocelle (co-advised with S. Patrick Walton), Amrita Oak, Kevin Chen (co-advised with S. Patrick Walton)

CURRENT RESEARCH

Network analysis to identify novel targets for cancer. The goal is to elucidate the effect of elevated levels of free fatty acids (FFAs), specifically palmitate, on cellular function, given its association with a number of diseases. Analyzing the mutation, copy number variation and gene expression patterns of a literature-derived model of metabolic genes associated with glycolysis, fatty acid metabolism and fatty acid uptake in >9,000 primary or metastatic tumor samples from the multi-cancer datasets found prominent roles of fatty acid uptake and metabolism on the metastatic progression and poor prognosis of human cancers.

Biophysical mechanisms of palmitate-induced signaling and cytotoxicity. This project integrates molecular biology, biophysics, and cellular studies with molecular modeling to enhance our understanding of complex biological systems comprising of multiple interacting processes. Specifically we are studying the endoplasmic reticulum transmembrane protein kinase/ endoribonuclease (IRE1), which is activated in response to the Unfolded Protein Response (UPR). This has broad implications on a number of diseases, since UPR is known to be activated in cancers, viral infection and many other diseases.

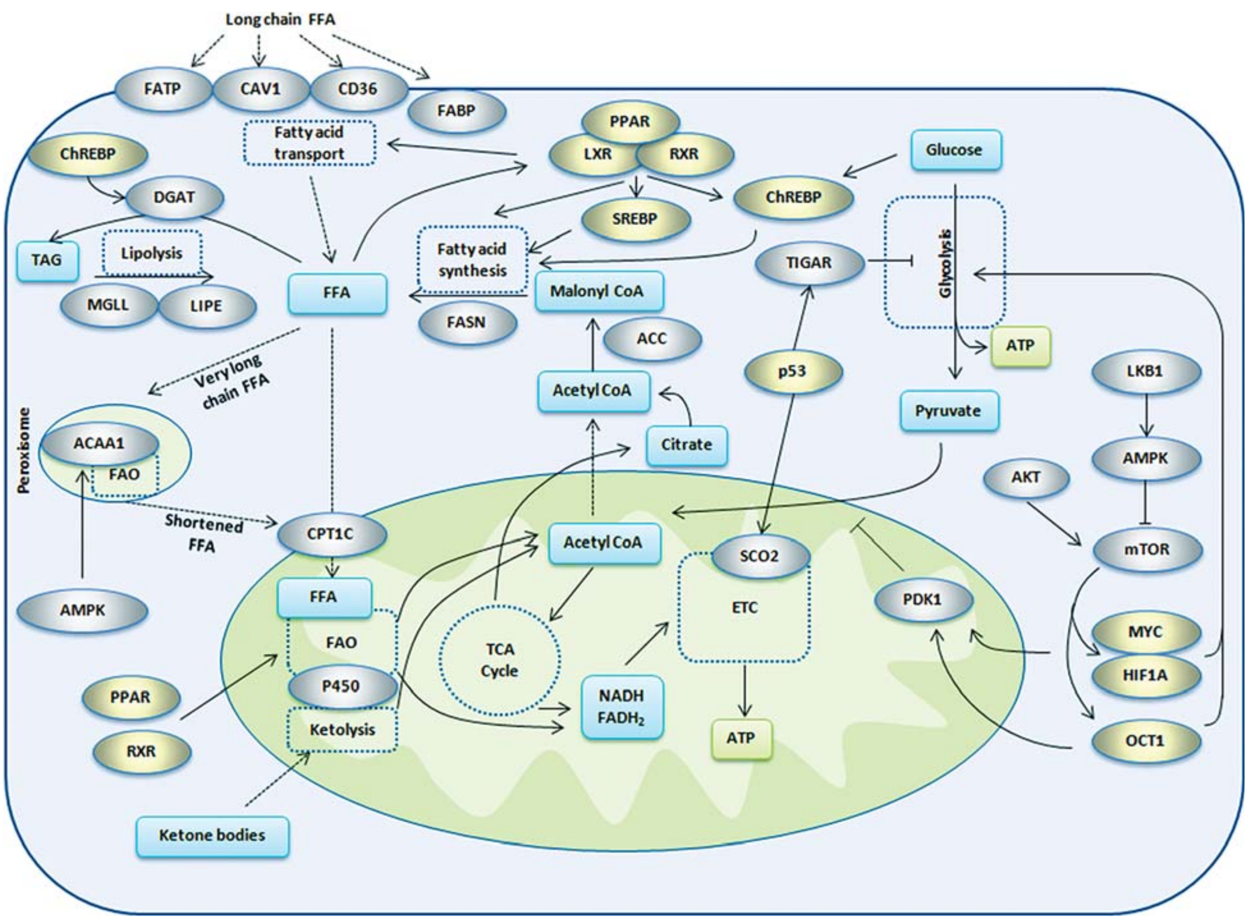

FIGURE 1. Literature-derived metabolic pathway model showing the genetic alterations that control glucose and fatty acid metabolism in cancer cells. The genes affecting FA transport were included in the pathway as potential contributors to the FA pool. FATPs indicate FATP1-6, FABPs indicate FABP1-9, and PPARs indicate PPAR-α, -δ and -γ. Silver ovals = proteins/enzymes, gold ovals = transcription factors, blue box = metabolites, dashed lines = transport, yellow box = ATP.

Delivery of siRNAs by polymeric nanoparticle (Collaborator: S. Patrick Walton). The overall goal of the proposed research is to design vehicles with optimal chemical and physical characteristics. The interactions of siRNAs with delivery vehicles built from chemically-diverse oligomeric and polymeric nanoparticles are quantitatively analyzed to determine those structural features that encourage complex formation and release of siRNAs into the cell.

Role of anisotropy on axonal growth and myelination. Mechanical cues play important roles in guiding various cell behaviors, such as cell alignment, migration, and differentiation. We found culturing DRG neurons for two weeks on stretched wherein purified Schwann cells were subsequently added showed significant myelination of the axons (overlap) of β-III-tubulin (green-axon) with P0 (red-myelination) over the unstretched surfaces.

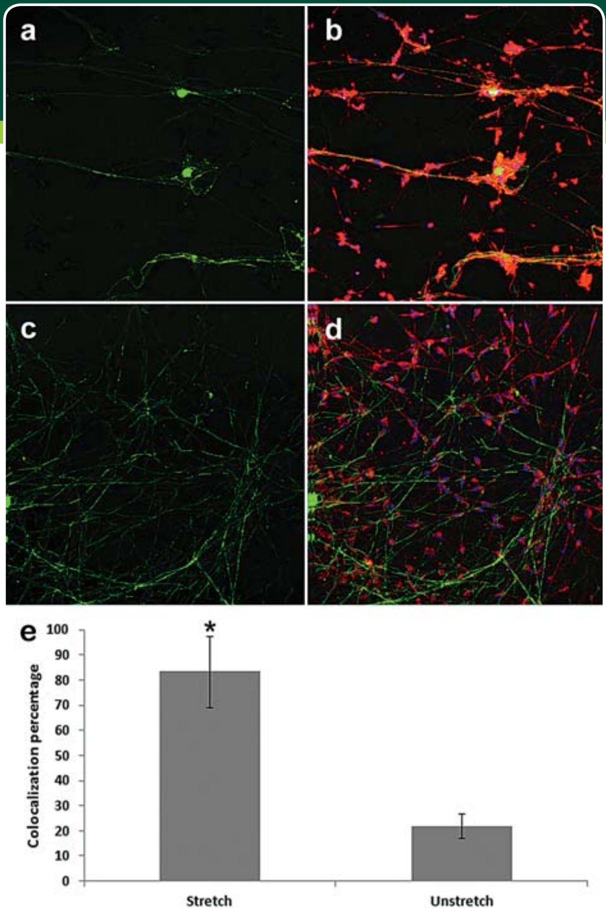

FIGURE 2. Co-cultured of Schwann cells with the DRG neurons on the stretched vs.unstretched PDMS substrates.

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D.A. Lynam, D. Shahriari, K.J. Felger, P.A. Angart, J. Koffler, M.H. Tuszynski, C. Chan, S.P. Walton, J. Sakamoto. "Brain derived neurotrophic factor release from layer-by-layer coated agarose nerve guidance scaffolds," *Acta Biomaterialia*, 18:128–31 (2015).

C.A. Kowalsky, M.S. Faber, A. Nath, H.E. Dann, V.W. Kelly, L. Liu, P. Shanker, E.K. Wagner, J.A. Maynard, C. Chan, T.A. Whitehead. "Rapid fine conformational epitope mapping using comprehensive mutagenesis and deep sequencing," *Journal of Biological Chemistry*, 290(44):26457-70 (2015). (doi: 10.1074/jbc.M115.676635)

C. Costello, NCI DREAM Community, et al. "A community effort to assess and improve drug sensitivity prediction algorithms." *Nature Biotechnology*, 32:1202–12 (2014). (doi:10.1038/nbt.2877)

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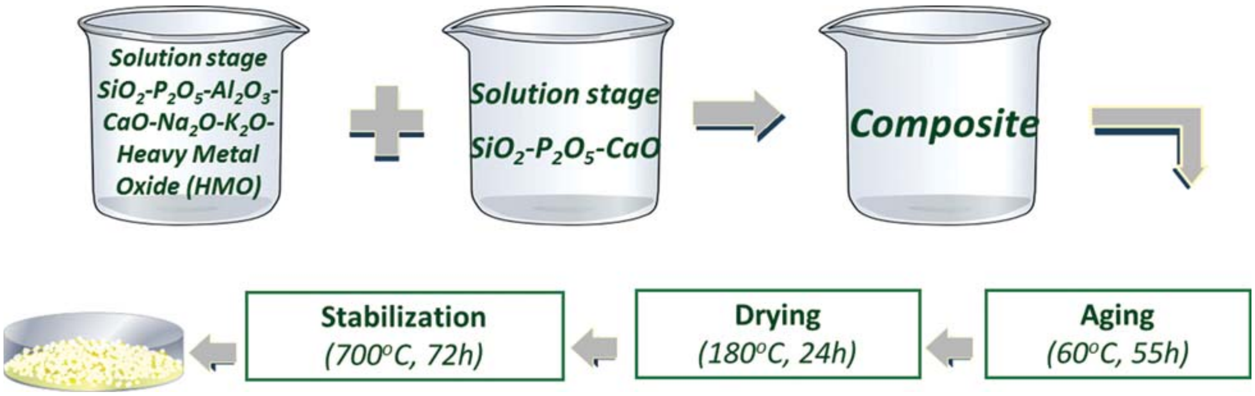

FIGURE 1. Illustration of the sol-gel method for particle fabrication.

RESEARCH INTERESTS

Bioactive glasses and glass-ceramics for combating bacteria and regeneration of lost, damaged, or diseased tissue. Sol-gel (solution-gelation) derived bactericidal and bioactive nano-particles, injectable composites with natural and synthetic hydrogels, 3D scaffolds, nanopatterned coatings on implants.

LAB

Bioactive glasses and glass-ceramics (3531 Engineering Bldg.)

GROUP

PHD STUDENT: Natalia Pajares Chamorro

CURRENT RESEARCH

Bioactive and bactericidal particles in nano and micro size. In this project, we apply the sol-gel method to fabricate bioactive glass-ceramic particles at micro and nano size.

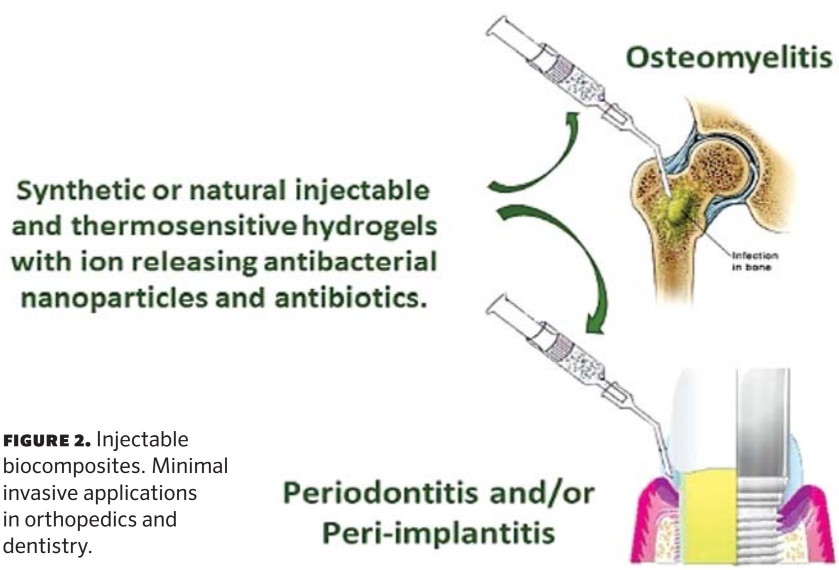

FIGURE 2. Injectable biocomposites. Minimal invasive applications in orthopedics and dentistry.

Different compositions with various antibacterial agents such as Ag, Zn, Cu, Se will be fabricated and compared in terms of their bacteriostatic or bactericidal activity. The particles will be further functionalized with antibiotics and the synergistic effect with the heavy metal ions will be studied. The bactericidal action will be observed against Methicillin-resistant *Staphylococcus aureus* (MRSA) and Vancomycin Resistant Enterococci (VRE). Their cell-material interaction will be studied in contact with hard and soft tissue for bone and dental tissue regeneration.

Injectable bioactive composites for minimal invasive applications in orthopedics and dentistry. The aim of this project is to develop systems that could accelerate the translation of the bactericidal and bioactive particles to the clinical practice. Synthetic microbeads made by alginate or collagen/fibrin as well as thermosensitive naturally derived extracellular matrix hydrogels (ECMs) will be applied as the delivery vehicle for the bioactive and antibacterial agents. The microstructural characteristics, antimicrobial action, regenerative properties and cytotoxicity of the developed injectable bio-composites will be studied in vitro and in vivo.

Nanopatterned 3D scaffolds. The sol-gel foam technique is applied for the fabrication of 3D scaffolds with macroporous structure ~300μm and interconnected mesoporous ~80μm. The scaffold surface is modified by functionalized antibacterial nanoparticles. The microstructural, morphological, mechanical, and bactericidal properties are studied. The biological properties are studied both in vitro and in vivo. The goal of this work is to fabricate advanced bioactive and antibacterial glass scaffolds that can provide a 3D hierarchical porous structure to better attract and regenerate lost or damaged tissue, while it will combat bacteria using a mechanism of action that bacteria cannot develop resistance to.
Nanopatterned coatings on implants. Sol-gel nanopatterned

bioactive coatings releasing metal ions and antibiotics (e.g., gentamicin, cefazolin, or vancomycin) for combined synergistic effects will be fabricated on different substrates, which are currently used as implants in different applications both in orthopedics and dentistry. The aim is to develop advanced bioactive and antibacterial coatings on the surface of implants. Dip coating is the applied method and the nano-patterned morphology is induced by using specific templates. The bond strength and the microstructural properties of the fabricated coatings at the interface are studied. The loading and delivery properties of the therapeutic drugs are also measured. Finally, the capability of the fabricated coatings to exhibit antimicrobial (ISO 22196:2011) properties and inhibit biofilm formation as well as the cell-coating interaction with hard and soft tissue are studied.

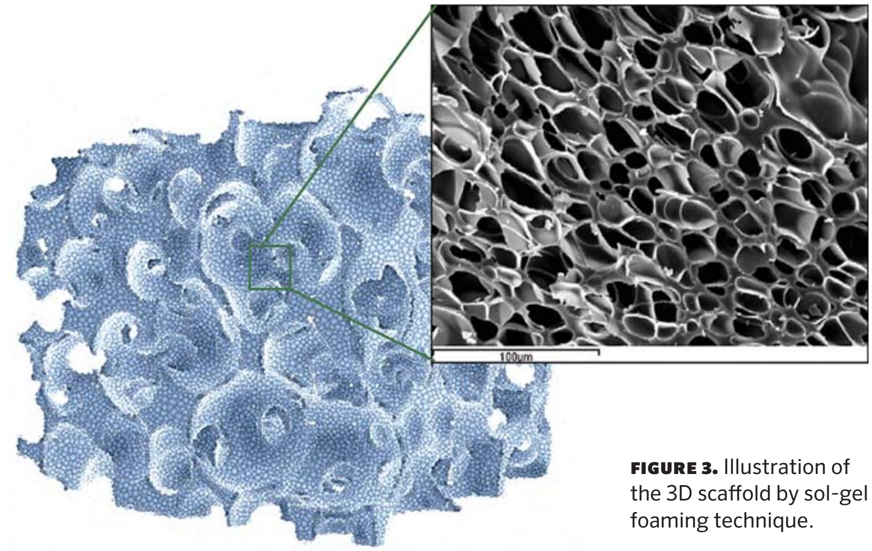

FIGURE 3. Illustration of the 3D scaffold by sol-gel foaming technique.

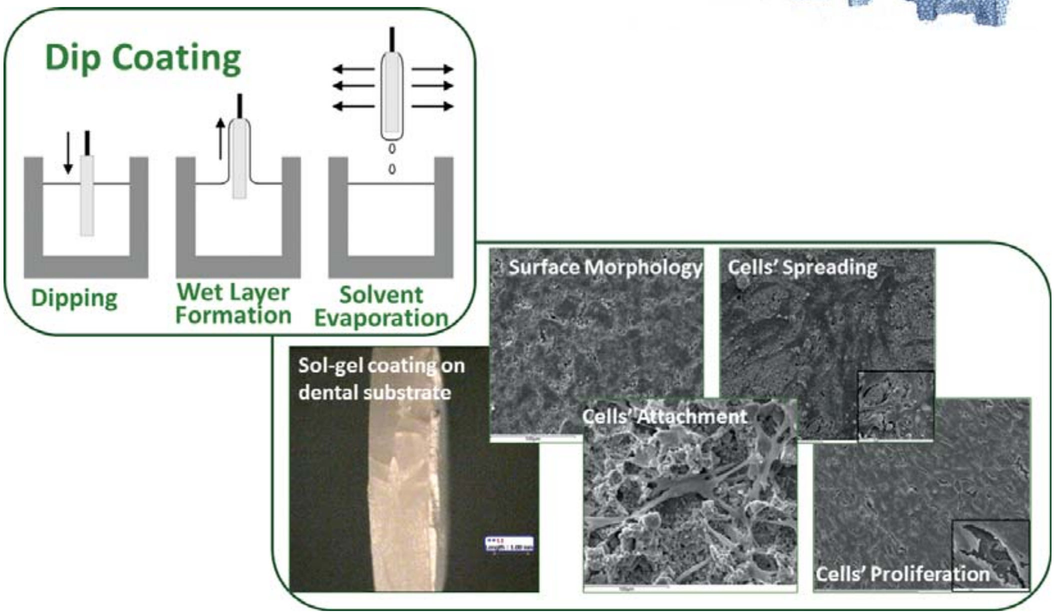

FIGURE 4. Sol-gel derived coating on dental ceramic substrate.Cell-coating interaction for applications in dentistry.

RECENT PUBLICATIONS

X. Chatzistavrou, R. R. Rao, D. J. Caldwell, A. W. Peterson, B. McAlpin, Y. Wang, L. Zheng, J. C. Fenno, J. P. Stegemann, P. Papagerakis, "Collagen/fibrin microbeads as a delivery system for Ag-doped bioactive glass and DPSCs for potential applications in dentistry," *Journal of Non-Crystalline Solids* 432, 143–149 (2016).

H. Kattan*, X. Chatzistavrou*, J. Boynton, J. Dennison, P. Yaman, P. Papagerakis, "Physical properties of an Ag-doped bioactive flowable composite resin, *Materials* 8.8, 4668–4678 (2015).

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Y. Wang*, X. Chatzistavrou*, D. Faulk, S. Badylak, L. Zheng, S. Papagerakis, L. Ge, H. Liu, P. Papagerakis, "Biological and bactericidal properties of Ag-doped bioactive glass in a natural extracellular matrix hydrogel with potential application in dentistry," *European Cells & Materials* (eCM) 29, 342–355 (2015).

X. Chatzistavrou, C. Fenno, D. Faulk, S. Badylak, T. Kasuga, A.R. Boccaccini, P. Papagerakis, "Fabrication and characterization of new bioactive and antibacterial composites for dental applications," *Acta Biomaterialia* 10, 3723–3732 (2014).

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RESEARCH INTERESTS

Materials deformation and fracture, substructure characterization, nanoindentation, grain boundary strain transfer, electron diffraction and channeling, dislocation mapping, scanning electron microscopy, transmission electron microscopy

LABS

Electron Microscopy and Characterization (3507 EB)
Sample Preparation Facilities (3510 EB)

WEBSITE

http://www.chems.msu.edu/people/profile/crimp

SPECIAL EQUIPMENT AVAILABLE

Three field emission scanning electron microscopes with electron backscattered diffraction (EBSD) orientation mapping capabilities, including one dual column focused ion beam (FIB)/FEG-SEM; tensile, bending, and high cycle fatigue in-situ deformation stages; heating and cooling stages

GROUP MEMBERS

POSTDOC: Shanoob Balachandran Nair. PH.D. STUDENTS: Su Yang, Bret Dunlap, Hank Han. UNDERGRADUATE STUDENTS: Elissa Klopfer, Daniel Branski

RECENT ACHIEVEMENTS

M.A. Crimp, "FIB Based Tomography of Dislocations Structures using Channeling Imaging," funded by the National Science Foundation, award $320,000, (7/1/2015–6/30/2017)

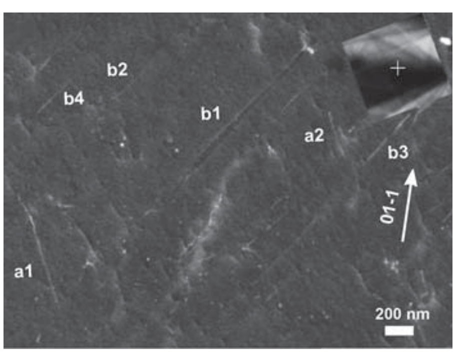
P. Eisenlohr, M.A. Crimp, T.R Bieler, "Systematic Identification of Constitutive Parameters for Crystal Plasticity Models of Non-Cubic Metal Alloys," funded by the National Science Foundation, award $419,916 (7/1/2014–6/30/2017).

C. Boehlert, T.R. Bieler, M.A. Crimp, P. Eisenlohr, "Characterization and Modeling of Deformation Induced Damage in Titanium Alloys," funded by the Dept. of Energy, Basic Sciences Division, total award $609,595 (9/15/15–9/14/2018).

CURRENT RESEARCH

The overall focus of this group is to develop and apply advanced electron beam characterization techniques. The group works on a range of interdisciplinary projects that deal with diffraction based imaging approaches, based on both scanning electron microscopy (SEM) and transmission electron microscopy (TEM). While the core research programs in this group deal with advancing the understanding of deformation and fracture in structural metals, collaborative studies have included magnetic multilayer structures, carbon nanotubes, ceramic joining, oxygen sensors, and cholesterol.

Characterization of deformation structures using scanning electron microscopy (with H. Mansour, J. Guyon, N. Gey, and N. Maloufi). Enhancing the performance of metals and alloys used in structural applications requires an understanding of the mechanisms that lead to strength, toughness, and in particular, damage nucleation that leads to failure. For many years these mechanisms have been characterized using TEM, but this approach is limited by the need to use very thin samples with small fields of views. Here at MSU we have been at the forefront in the development of SEM approaches that allow the direct imaging and crystallographic characterization of deformation structures in the near surface regions of bulk samples using electron channeling contrast imaging (ECCI) (Figure 1). Critical to these studies is the ability to determine crystal orientation with high accuracy (with 0.1°). While many crystallographic studies in SEM are carried out using EBSD (and we do use this approach extensively), it does not meet the stringent requirements for imaging deformation structures. Rather, selected area channeling patterns (SACPs), historically with spatial resolutions in the range of 10–20 μm, are required for setting up imaging conditions. We have developed a new approach for collecting high resolution SACPs, with spatial resolutions better than 0.5 μm (Figure 2). While facilitating characterization of deformation structures in fine grain materials, this approach also allows highly accurate misorientation measurements across grain boundaries



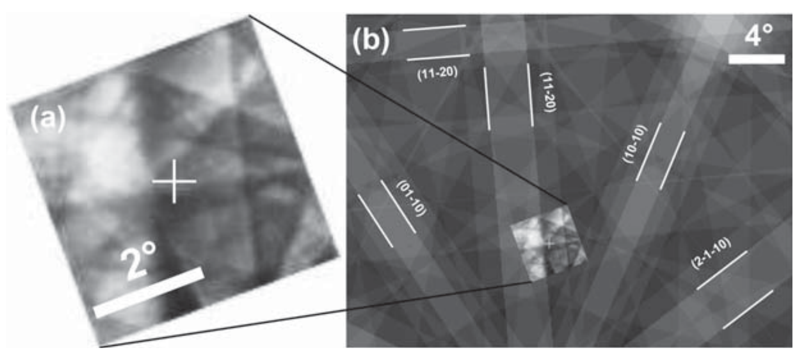
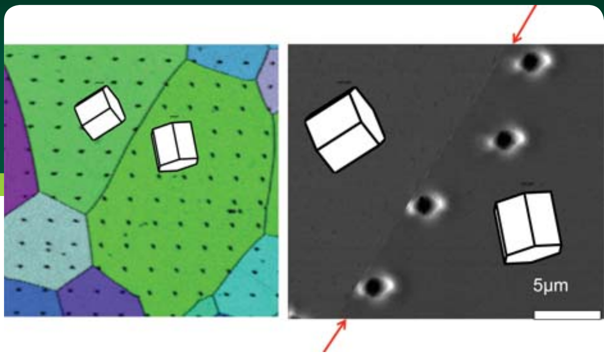


FIGURE 1 (*left*). Deformation structure in interstitial steel showing screw dislocations following 2% plastic strain. **FIGURE 2 (*right*).** (A) HR-SACP collected from a sub-micron region of an IF steel, allowing highly accurate imaging of crystal defects. (B) HR-SACP superimposed on a simulated pattern show imaging conditions in relation to other channeling bands.



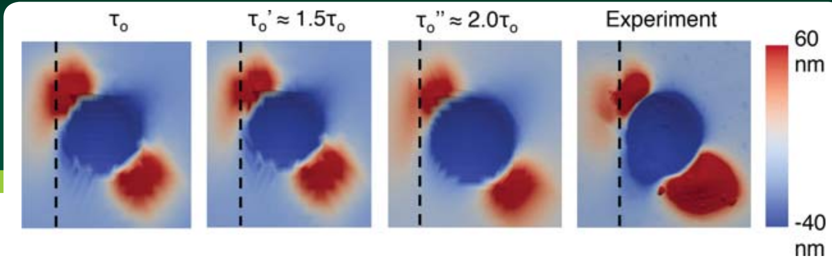


FIGURE 3 (*left*). *LEFT:* EBSD map of crystal orientations showing nanoindentations. *RIGHT:* High magnification AFM image showing topography changes as the indentations move close to a grain boundary.
FIGURE 4 (*above*). Plastic deformation simulations of nanoindentation topography with varying slip resistant at the grain boundary compared with the experimentally measured topography development.

and dislocation cell walls. Combined with analysis of ECCI image characteristics, this high accuracy technique allows determination of both geometrically necessary and statistically stored dislocations (GNDs and SSDs) in deformed structures.

Characterization and modeling of anisotropic deformation in polycrystals (with T. Bieler, C. Boehlert, P. Eisenlohr, and C. Zambaldi). While the mechanisms associated with plastic deformation of single crystals are very well established, the manner in which these mechanisms facilitate the shape changes needed to simultaneously deform the various grains in a polycrystal are not well understood. If different grains cannot mutually accommodate imposed strain, performance-limiting nucleation of void/cracks may develop. This research program is using EBSD and ECCI in combination with plastic deformation simulations to characterize polycrystalline deformation and damage nucleation. We carry out nanoindentation experiments and complementary simulations to (1) determine the critical parameters for simulating plastic deformation in single crystals and (2) quantify how grain boundaries limit the strain transfer from one grain to the next. Figure 3 shows an EBSD orientation map with a series of nanoindentations, along with, along with atomic force microscopy (AFM) topography maps of nanoindentation taken close to and far from a grain boundary. The topography of the indentations is truncated by the boundary, indicating the boundary resists the transfer of strain from one grain to the other. Figure 4 shows a series of simulated nanoindentation topographies in comparison with the experimentally measured topography. As the resistance to slip of the grain boundary increases from a from single crystal slip resistance of $\sigma_o = 1.0$ to $\sigma_o = 2.0$, the topography in the receiving grain decreases and more accurately reflects the experimentally measured topography. The grain boundary slip parameters are found to change for different classes of grain boundaries. These results are being incorporated in to plasticity simulations of polycrystalline arrays to evaluate if the experimentally measured strains can be accurately matched. ECCI has been used to image the dislocation structures around nanoindents, and compared to GNDs mapped using cross-correlation EBSD, the first time such studies have been carried out.

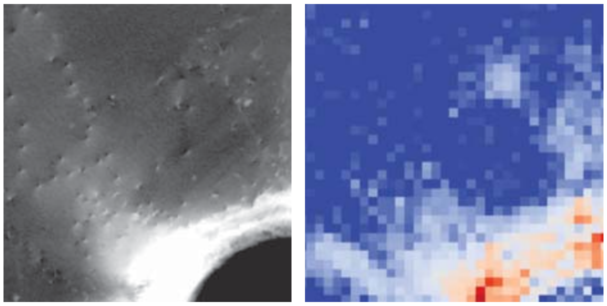


FIGURE 5. ECC image of dislocation distribution around a nanoindents (*left*) and cross-correlation EBSD map of the showing GND distribution.

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RESEARCH INTERESTS

Energy and sustainability, food and energy, cellulosic biofuels, life cycle assessment

LAB

Biomass Conversion Research Laboratory

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SPECIAL EQUIPMENT AVAILABLE

Pretreatment of cellulosic biomass using ammonia, full lab capabilities in pretreatment, hydrolysis, and fermentation of cellulosic biomass; strong capabilities in life cycle assessment for biofuels and bioproducts

GROUP MEMBERS

Professor Venkatesh Balan, Professor Seungdo Kim, Dr. Leonardo da Costa Sousa, Dr. Somnath Shinde, Ms. Saisi Xue, Mr. Linchao Zhou, Mr. Thapelo Mokomele.

PATENTS

"Extraction of Solubles from Plant Biomass for Use as a Microbial Growth Stimulant and Methods and Systems Related Thereto." Australia Patent 2011201768. (2014)

"Pretreated Densified Biomass Products." US Patent 8,673,031. (2014)

"Extraction of Solubles and Microbial Growth Stimulants from Lignocellulosic Biomass and Methods Related Thereto." US Patent 9,206,446. (2015)

"Methods for Producing and Using Densified Biomass Products Containing Pretreated Biomass Fibers." US Patent 9,039,792. (2015)

RECENT ACHIEVEMENTS

Continuing support from the Department of Energy, Great Lakes Bioenergy Research Center

Michigan Technology and Research Commercialization Program

Elected a Fellow of the American Institute of Medical and Biological Engineers (2015)

Elected Fellow of the National Academy of Inventors (2014)

CURRENT RESEARCH

Sustainable biofuels and bioproducts. The U.S. Congress passed the Renewable Fuels Standard (RFS) seven years ago. Since then, biofuels have gone from darling to scapegoat for many environmentalists, policy makers, and the general public. The reasons for this shift are complex and include concerns about environmental degradation, uncertainties about impact on food security, new access to fossil fuels, and overly optimistic timetables. As a result, many people have written off biofuels. However, numerous studies indicate that biofuels, if managed sustainably, can help solve pressing environmental, social, and economic problems (Figure 1). The scientific and policy communities as well as the general public should take a closer look by reviewing the key assumptions underlying opposition to biofuels and carefully consider the probable alternatives. Liquid fuels based on fossil raw materials are likely to come at increasing environmental cost. Sustainable futures require energy conservation, increased efficiency, and alternatives to fossil fuels, including biofuels.

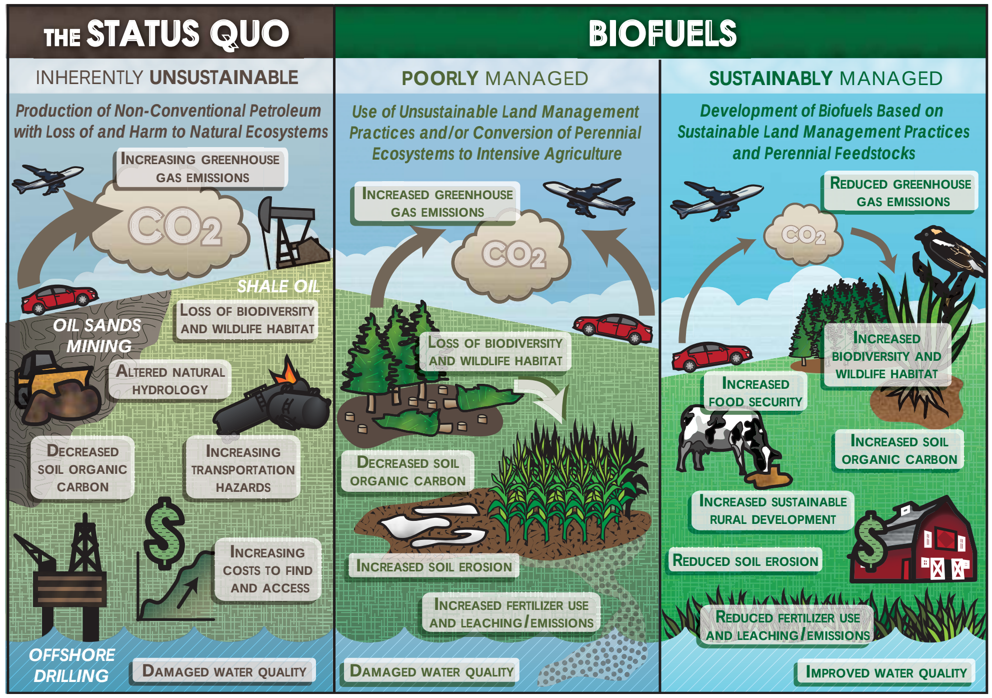
Access to high-quality energy sources is strongly linked to prosperity and human well-being. Economies benefit when they produce biofuels, a dynamic observed in both developed and developing nations. Indigenous biofuel production increases energy security. Producing perennial biofuel feedstocks can improve water and soil quality, biodiversity, and wildlife habitat compared to landscapes dominated by annual crops. Biofuels can also enhance rural employment and food security. Because photosynthesis consumes CO_2 and because perennial crops can accumulate soil carbon, biofuel production and utilization can be carbon neutral and even reduce net atmospheric CO_2. Thus, low-carbon energy scenarios developed by diverse organizations foresee widespread use of biomass for energy (Figure 2). Biomass provides an average of 138 exajoules of primary energy across these five scenarios, or about one-quarter of total global primary energy. These scenarios use biomass primarily to satisfy energy needs that likely cannot be met by other renewables. For example, aviation and ocean shipping require liquid fuels and liquid fuels are strongly preferred for long-haul trucking. Biofuels are only one part of a sustainable energy portfolio, but it is highly unlikely that we can achieve a sustainable transportation sector without biofuels.

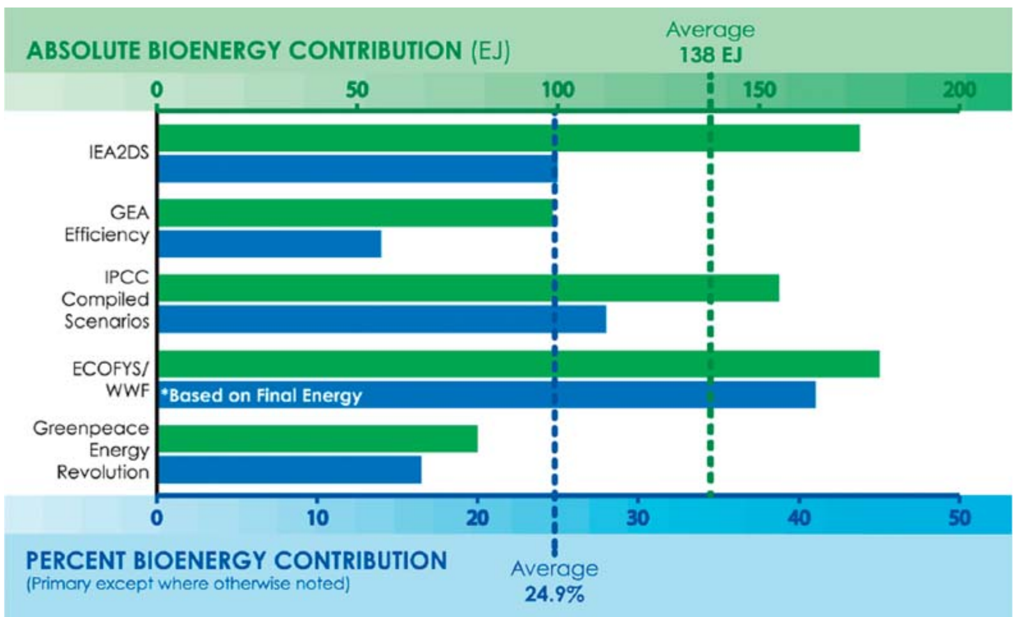
Many materials used by society can be recycled, but fossil fuels cannot. Economic activities based on massive fossil fuel consumption are therefore inherently unsustainable. Extracting and using oil, natural gas, and coal exposes humankind to air and water pollution and to escalating climate challenges. Thus, both economic self-interest and ethical considerations require that we develop sustainable alternatives to fossil fuels, including biofuels.

Progress toward more sustainable energy sources requires continual improvement in meeting current energy needs while preserving options for the future. For example, biofuels should be integrated with sustainable agriculture and forestry systems. Managing such systems requires ongoing assessment to identify better options. The complete system (feedstock production, logistics, conversion technologies, energy types, coproducts, transport and delivery systems, and engine or power technology) must be compared to alternatives, including fossil fuels. Stakeholder engagement in developing and evaluating sustainability attributes is critical. Stakeholders determine baseline comparisons, consequential effects and how tradeoffs, synergies, and targets evolve. Following this approach, a broadly endorsed "win-win" role for perennial biomass crops was recently established in the United Kingdom.

Biofuels are relevant as the U.S. and other nations develop energy and climate policies. More sustainable biofuel production pathways today allow society to better meet tomorrow's climate and energy goals. Economic and geopolitical concerns are strongly influenced by energy resources. A nation that develops renewable energy options is stronger and more resilient over the long-term.

Sustainably deployed biofuels can contribute to solving challenging problems, including food and energy security, climate change and environmental degradation caused by current agricultural and forestry practices. While the desirable outcomes of sustainable biofuel production and use are not guaranteed, they are certainly achievable. In contrast, it is very difficult to see how continued massive reliance on liquid fuels from fossil materials can achieve positive environmental outcomes, especially higher carbon options such as oil sands, deep water drilling, natural gas-to-liquids and coal conversion. Thus, biofuels deserve a closer look. Sustainably deployed biofuels help can help society achieve many "win-wins" by supporting important environmental, economic, and social goals.





RECENT PUBLICATIONS

B.E. Dale, J. Anderson, R. Brown, S. Csonka, V. Dale, G. Herwick, R. Jackson, N. Jordan, S. Kaffka, K. Kline, L. Lynd, C. Malmstrom, R. Ong, T. Richard, C. Taylor, M.Q. Wang. "Take a closer look: biofuels can support environmental, economic and social goals," *Environmental Science and Technology* 48: 7200–7203 (2014).

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B.E. Dale, M.T. Holtzapple. "The need for biofuels," *Chemical Engineering Progress.* March 2015. pp. 36–40.

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S. Kim, B.E. Dale. "All biomass is local: The cost, volume produced, and global warming impact of cellulosic biofuels depend strongly on logistics and local conditions," *Biofuels, Bioprod. Bioref.* (2015). (doi: 10.1002/bbb.1554)

S. Pattathil, M.G. Hahn, B.E. Dale, S.P.S. Chundawat. "Insights into plant cell wall structure, architecture, and integrity using glycome profiling of native and AFEX-pretreated biomass," *Journal of Experimental Botany*, Vol. 66, No. 14: 4279–4294 (2015). (doi:10.1093/jxb/erv107)

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RESEARCH INTERESTS

Polymer-fiber composite materials, nano-composites (graphene, halloysite, silica), bio-composites (bast fibers, cellulose nano-fibrils, cellulose nano-whiskers), fiber-polymer interfaces (carbon, glass uhmwpe, aramid), adhesion, adhesive bonding, nanostructured electrodes for batteries and supercapacitors

LAB

Composite Materials and Structures Center

WEBSITES

http://www.chems.msu.edu/people/profile/drzal
www.egr.msu.edu/cmsc

SPECIAL EQUIPMENT AVAILABLE

Specific instrumentation available for the fabrication, evaluation, characterization and testing of polymer, fibers, nanoparticles and their polymer composite materials:

- COMPOSITE MATERIALS EVALUATION AND ANALYSIS
  Zeiss Environmental Scanning Electron Microscope (ESEM) integrated with a Dual Beam Focused Ion Beam (FIB), X-ray Photoelectron Spectroscopy PerkinElmer 5400, Contact Angle Krusse Dynamic Measurement System, Contact Angle Cahn Microbalance, Thermal Analysis TA 2900 Instruments (DSC, TGA, TMA, DTA), Rheological Analysis TA Instruments AR2000X Rheometer, AFM-Scanning Probe Microscopy (Nano Scope IV), Nano-Indentation-MTS, Permeability Mocon Permeability System (water, CO_2, O_2), Thermal Conductivity System Anter Unitherm 2022, Ultramictrotomy RMC-MT7, Ultrasoncinator Heilsher 1000W pulsed system, Potentiostat/Galvanostat Measurement Applied Research VMC-2 Versastat System, Inert Fabrication Glovebox MBRAUN Unilab 2000/780 Argon Glovebox, Plasma Surface Modification Plasma Sciences 500 Surface Treatment plasma reactor, UV Light Source: Xenon RC 747 HVPS system, Rheometer: TA Instruments AR2000ex, ARES, Viscometer-Brookfield, Netzsch Xenon Flash Thermal conductivity units
- COMPOSITE MATERIALS FABRICATION
  Cryo-Mill Mikro-Bantam Model CF, C.W. Brabender 85cc Banbury Mixer, Labram Vacuum Mixing System, Sweco Vibro-Energy Grinding Mill, Exact Three Roll Mill, Microwave Synthesis Milestone ETHOS EZ Microwave Labstation, Tetrahedron Programmable Smart Press (40 ton, Double Daylight, Temp 1000°F, Programmable Temp and Pressure), Leistritz Micro-27 Twin Screw Extruder System and related auxiliary equipment, DSM Research 15 cc Micro-extruder (two units), Killion 75-in Single Screw Extruder, Cincinnati Milacron Sentry 85 Injection Molder, United McGill Autoclave, Research Tool Hot-Melt Prepregger (two units), Research System Resin Transfer Molding

GROUP MEMBERS

PHD STUDENTS: Deandrea Rollins, Markus Downey, Keith Honaker-Schroeder, Mariana Batista, Zeyang Yu

SELECTED PATENTS (35 TOTAL)

"Nanoparticle graphite-based minimum quantity lubrication method and composition," P. Kwon, L.T. Drzal. US Patent 9,080,122 B2 (7/14/2015).

"Micropatterning of conductive graphite particles using microcontact printing," I. Lee, L.T. Drzal, J. Lu. US Patent 9,023,478 (5/5/2015).

"Method for the preparation of doped single graphene sheets," L.T. Drzal, I. Do, A. Monga. US 20130337351 A1 (12/19/2013).

"Method for preparing metal nanoparticles," L.T. Drzal, I. Do. WO/2013/049433 PCT/US2012/057694.

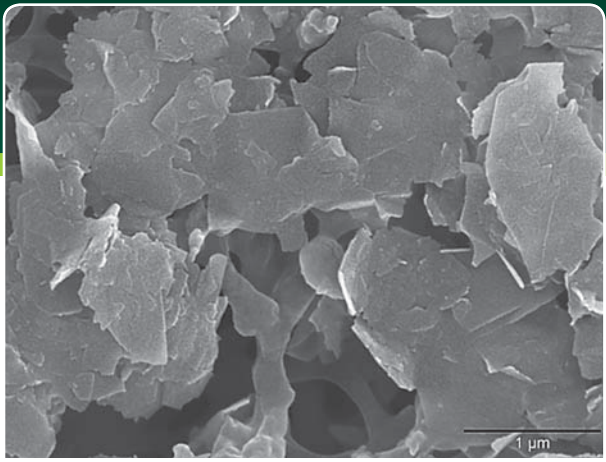
"Expanded graphite and products produced therefrom," L.T. Drzal, H. Fukushima. US Patent 8,501,858 (8/6/2013).

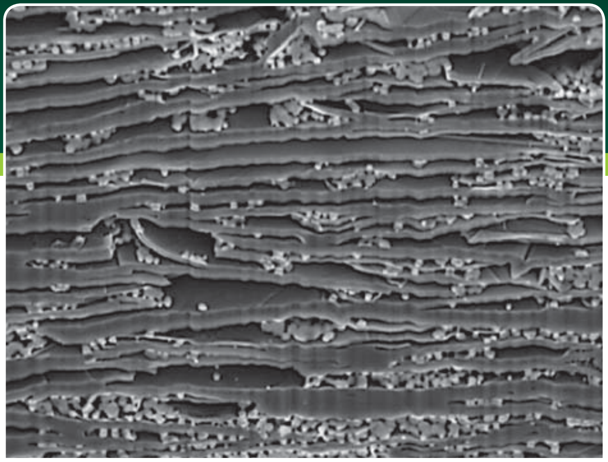
"Conductive composite compositions with fillers," L.T. Drzal, W. Liu, H. Fukushima, I. Do. US Patent 8,017,228 B2 (9/13/2011).

CURRENT RESEARCH

Nanostructuring of multifunctional graphene nano-platelet composites for structural, energy generation and energy storage applications. The Drzal research group is in general conducting research in polymer composites including: polymer composites reinforced with fibers and nanoparticles (graphene and cellulose), processing of composites, adhesion, biobased composites, and the nanostructuring of these materials in polymers for structural and energy generation and storage applications. He is also co-founder and Chief Scientist of XG Sciences, Inc., a Michigan-based start-up company to produce graphene nanoplatelets. Specific ongoing projects include:

Investigation into the enhancement of polymers with graphene nanoplatelets. The objective of this project is to develop the next generation of aerospace structural multifunctional materials (polymer + fiber + nano particle) that will provide a balance between processing and performance. It is envisioned that an aerospace polymer composite compound will be developed which is modified with graphene nanoplatelets at various concentrations to provide a material optimized for: (1) strength and modulus, (2) electrical conductivity, (3) thermal conductivity, and (4) thermal expansion. This will involve extrusion processing and nanostructuring of the nanoparticles into highly aligned films for integration into composites.

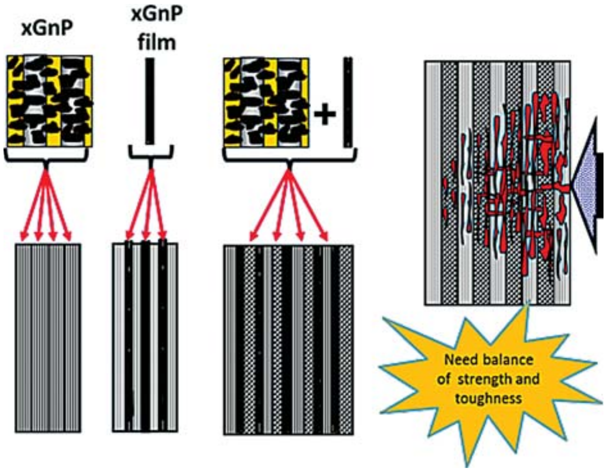




Nano-structured materials for Li ion battery and supercapacitors. The objective of this research project is to: (1) gain a fundamental understanding of the atomic and molecular level processes that govern the operation, performance and failure mechanisms of energy storage systems; (2) design and investigate nanostructured materials with the goal of increasing the performance, durability and reliability of batteries and supercapacitors; (3) explore nanostructuring of materials for battery and supercapacitor materials to facilitate fast electron and ion transport with an emphasis on high power and high capacity batteries for electric vehicles.

Drzal's portion of the project involves the nanostructuring of graphene nanoplatelets in the anode to improve capacity, re-charging rate and durability.

Multifunctional composite materials. The objectives of the research are: (1) to demonstrate a new approach to improving composite fracture and impact toughness by surface modification and coating with functionalized elastomeric coatings of nanoparticles and (2) to impart flammability improvement and flame resistance by the incorporation of xGnP into structural composite materials. The primary focus is on glass and carbon fiber reinforced vinyl ester composites used as structural elements in Army ground vehicles. The insertion of xGnP nanoparticles around fibers and between lamina in a composite can deflect blast and impact energy laterally away from the impact point and provide a safety margin by preventing structural collapse.



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F. Wang, L.T. Drzal, Y. Qin, Z. Huang. "Size effect of graphene nanoplatelets on the morphology and mechanical behavior of glass fiber/epoxy composites," *J. Materials Science*, 51:3337–3348 (2016). (doi 10.1007/s10853-015-9649-x)

N.T. Kamar, M.M. Hossain, A. Loos, L.T. Drzal. "Interlaminar reinforcement of glass fiber/epoxy composites with graphene nanoplatelets," *Composites, Part A*, 70, 82–92 (2015).

F. Wang, L.T. Drzal, Y. Qin, Z. Huang. "Mechanical properties and thermal conductivity of graphene nanoplatelet/epoxy composites," *J. Materials Science*, 50, 1082–1093 (2015).

W. Qin, F. Vautard, L.T. Drzal, J. Yu,. "Mechanical and electrical properties of carbon fiber composites with incorporation of graphene nanoplatelets at the fiber–matrix interphase," *J. Composites, Part B*., 69, 335–341 (2015).

W. Qin, F. Vautard, L.T. Drzal, J. Yu. "Modifying the carbon fiber-epoxy matrix interphase with silicon dioxide nanoparticles," *RSC Adv.*, 5 (4), 2457–2465 (2015).

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W. Bose, L.T. Drzal. "Functionalization of graphene nanoplatelets using sugar azide for graphene/epoxy nanocomposites," *Carbon Letters*, 16(2) 101–106 (2015).

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V. Cech, A. Knob, H.-A. Hosein, A.Babik, P. Lepcio, F. Ondreas, L.T. Drzal. "Enhanced interfacial adhesion of glass fibers by tetravinylsilane plasma modification," *Composites Part A: Applied Science and Manufacturing*, 58, 84–89 (2014).

Philip Eisenlohr

Associate Professor

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RESEARCH INTERESTS

Computational materials science, mechanics of microstructured materials, crystal plasticity

LAB

Computational Materials Mechanics (1260 Engineering Bldg.)

WEBSITE

compmatermech.wordpress.com

SPECIAL EQUIPMENT AVAILABLE

Dedicated computer clusters at the MSU High Performance Computing Center

GROUP MEMBERS

PHD STUDENTS: Tias Maiti, Aritra Chakraborty, Zhuowen Zhao, Eureka Pai Kulyadi, Mingwan Zhu. UNDERGRADS: Brendan Vande Kieft, Jacob Shereda

RECENT ACHIEVEMENTS

DoE-OHEP (2016): "The Effect of Process History on Grain Boundaries and Dislocation Substructures on Functional Properties of Nb for SRF Cavities: Plastic Formability and Microstructural Evolution," T.R. Bieler, P. Eisenlohr, N.T. Wright, C.C. Compton

DoE-BES (2015): "Characterization and Modeling of Deformation-Induced Damage in Hexagonal Metals," P. Eisenlohr, C.J. Boehlert, T.R. Bieler, M.A. Crimp DoE-BES (2015): "Characterization and Modeling of Deformation-Induced Damage in Hexagonal Metals," P. Eisenlohr, C.J. Boehlert, T.R. Bieler, M.A. Crimp

CURRENT RESEARCH

Computational prediction of advanced structural material performance by considering interactions of microstructure and plasticity in crystalline solids. In our daily life, we heavily rely on the mechanical capacity and integrity of many different materials. For most structural materials of technological relevance, the mechanical behavior is intricately influenced by their chemistry (alloying in the case of metals) but even more importantly by their microstructure. The latter is strongly impacted by processing conditions and, hence, can be substantially manipulated through processing. This complexity makes the prediction of the (thermo-) mechanical behavior of existing materials and the design of new materials and their required microstructures for targeted properties a remarkable challenge that is addressed at the Computational Materials Mechanics (CMM) lab by Eisenlohr and his group. We tap into the resources offered by the High Performance Computing Center (HPCC) and the Division of Engineering Computing Services (DECS) to simulate material deformation with commercial and homemade open-source so ware. In our simulations, we investigate the mechanisms of deformation occurring at mesoscopic scales and connect them to the material microstructure. By this we seek, for instance, to (1) understand basic aspects of plastic deformation in crystals, (2) identify critical configurations in polycrystals or multiphase materials that might trigger nucleation of internal damage, and (3) predict the inherently anisotropic behavior of structural materials with complex microstructure at the scale of engineering components.

As an overarching theme, we seek to advance the forward modeling and associated simulation methodologies necessary to understand the properties of materials with (complex) microstructure and by that facilitate the solution of the inverse problem posed by the search for a microstructure that meets a given property demand.

Examples for ongoing research are:

Relevance of grain neighborhood on polycrystalline plasticity. The mechanical response of multiphase metallic materials is governed by the strain and stress partitioning behavior among their phases, crystals, and subgrains. Despite knowledge about the existence of these complex and long-ranging interactions, the experimental characterization of such materials is often limited to surface observations of microstructure evolution and strain partitioning, i.e., ignoring the influence of the underlying features. Hence, for the interpretation of the observed surface behavior it is imperative to understand how it might be influenced by the subsurface microstructure. We therefore systematically varied the subsurface microstructure of synthetic dual-phase polycrystals and investigated the altered response of a 2D region of interest. The series of high-resolution crystal plasticity simulations are conducted with a fast and efficient spectral-based iterative scheme for calculating the mechanical response of complex crystalline materials. We could show that the subsurface microstructure up to a depth of about 3 to 4 grains has a dominant influence on the observed stress and strain partitioning. Furthermore, this zone of influence increases with increasing heterogeneity of the microstructure. This indicates that, especially for complex microstructures, surface observations are hard to interpret at the scale of individual grains when the underlying microstructure (particularly the phase distribution) is not known.

Systematic identification of constitutive parameters for crystal plasticity models of non-cubic metal alloys. The integration of computational modeling into process development and design continues to accelerate due the potential shortened development times, cost savings, and enhanced reliability. At the fundamental level, the controlling factors in the mechanical behavior of structural metals are the resistance of dislocations to slip, i.e., the critical resolved shear stress for the motion of dislocations, and the concurrent structural evolution (e.g. work hardening). Thus, in order to accurately describe the deformation, possible damage nucleation, and fracture behavior of the polycrystalline arrays that make up structural components, it is necessary to have a sound model with physical deformation processes involved and accurate values for the adjustable parameters that enter such models. Determining these constitutive parameters is quite challenging for technologically relevant materials of low crystal symmetry, such as Mg-alloys, Ti-alloys, or lead-free solders based on Sn.

We are presently investigating a newly developed approach to determine parameters of the constitutive description in a relatively rapid and cost effective manner by cono-spherical nano-indentation into a sufficiently large number of different crystal orientations at the surface of polycrystalline samples. Atomic force microscopy is then used to measure the topography around these indents, which is a strong function of the crystal orientation and the specific local activity of different slip systems. Crystal plasticity finite element simulation of the indentation process is then carried out with varying constitutive parameters until an optimal match is achieved between the measured and simulated topographies in several different indents on crystals with different orientations/topographies. This method is effective because the axisymmetric cono-spherical indentation geometry causes many different slip systems to operate at different rates and along different strain paths depending on the material location beneath the indent.

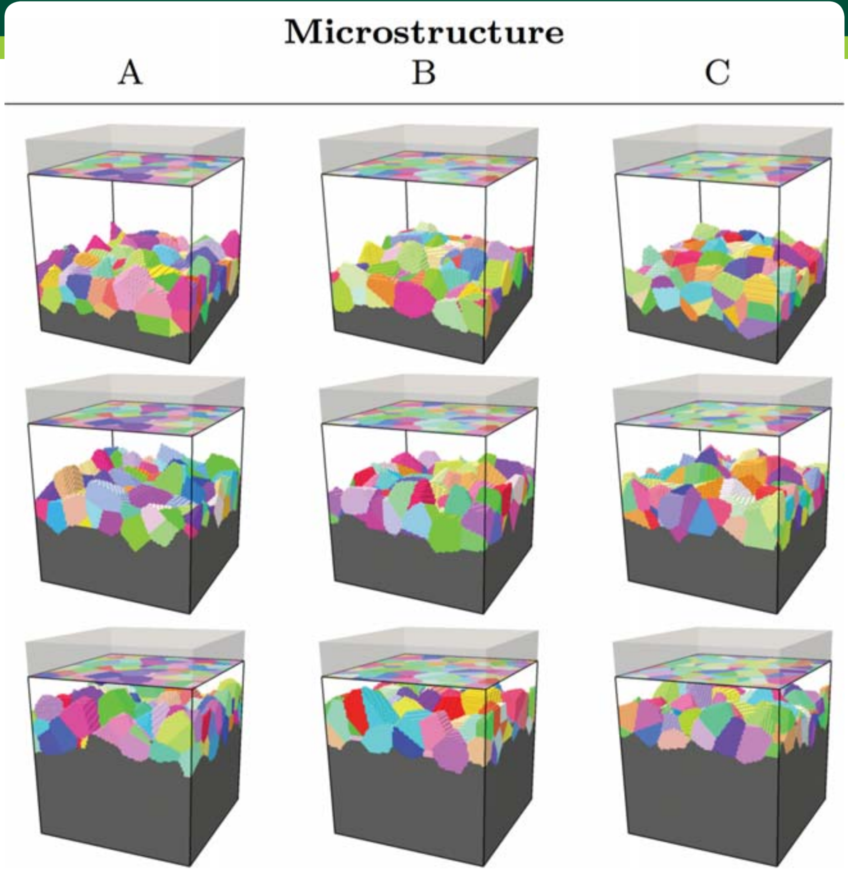

FIGURE. Periodic polycrystalline domains to study how an alteration of the crystal orientation within the colored layer influences the response observable at the (top) surface. Structure above and below of the layer (invisible and solid gray) remains unaltered.

RECENT PUBLICATIONS

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W. Blum, J. Dvořák, P. Král, P. Eisenlohr, V. Sklenička, "Effects of grain refinement by ECAP on the deformation resistance of Al Interpreted in terms of boundary-mediated processes," *J. Mater. Sci. Technol.*, 32(12), 1309–1320 (2016).

W. Blum, P. Eisenlohr, J. Hu, "Interpretation of unloading tests on nanocrystalline Cu in terms of two mechanisms of deformation," *Mater. Sci. Eng. A*, 665, 171–174 (2016).

M.Diehl, P. Shanthraj, P. Eisenlohr, F. Roters, "Neighborhood influences on stress and strain partitioning in dual-phase microstructures. An investigation on synthetic polycrystals with a robust spectral-based numerical method," *Meccanica*, 51(2), 429–441 (2016).

D. Ma, P. Eisenlohr, E. Epler, C.A. Volkert, P. Shanthraj, M. Diehl, et al. "Crystal plasticity study of monocrystalline stochastic honeycombs under in-plane compression," *Acta Mater.*, 103, 796–808 (2016).

Y. Su, C. Zambaldi, D. Mercier, P. Eisenlohr, T.R. Bieler, M.A. Crimp, "Quantifying deformation processes near grain boundaries in alpha-titanium using nanoindentation and crystal plasticity modeling," *Int. J. Plasticity* 86, 170–186 (2016).

X. Wu, D. Ma, P. Eisenlohr, D. Raabe, H.-O. Fabritius, "From insect scales to sensor design: modeling the mechanochromic properties of bicontinuous cubic structures," *Bioinspir. Biomim.*, 11(4), 045001– (2016).

W. Blum, J. Dvořák, P. Král, M. Petrenec, P. Eisenlohr, V. Sklenička, "In situ study of microstructure and strength of severely predeformed pure Cu in deformation at 573 K," *Philos. Mag.*, 95(33), 3696–3711 (2015).

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D. Ma, P. Eisenlohr, P. Shanthraj, M. Diehl, F. Roters, D. Raabe, "Analytical bounds of in-plane Young's modulus and full-field simulations of two-dimensional monocrystalline stochastic honeycomb structures," *Comp. Mater. Sci.*, 109, 323–329 (2015).

David Hodge

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RESEARCH INTERESTS

Bioenergy, biomass conversion, lignin, bio-based products

LAB LOCATION

28 Trout Building

WEBSITE

http://www.chems.msu.edu/groups/hodge/

GROUP MEMBERS

Ryan Stoklosa, Jacob Crowe, Thanaphong Phongpreecha, Lisaura Maldonado, Dhruv Gambhir, Guilong Yan, Pachara Sattayawat

PATENT

"Multi-ligand metal complexes and methods of using same to catalytically pretreat lignocellulosic biomass," D.B. Hodge, E.L. Hegg, Z. Li, A. Bhalla, N. Bansal. US Patent Application 20150352540 (2015).

RECENT ACHIEVEMENTS

RESEARCH SUPPORT FROM:

- Department of Energy, Great Lakes Bioenergy Research Center
- Michigan Translational Research and Commercialization (MTRAC)
- NSF CBET—Energy for Sustainability
- Northeast Sungrant

CURRENT RESEARCH

Conversion of plant-derived biomass to renewable fuels, chemicals, polymers, and materials. The long-term sustainability of human civilization will require non-fossil sources of both energy and carbon in the future as well as the technologies for their effective capture, storage, and conversion. Non-food plant biomass offers an immense reservoir of reduced carbon, which is primarily comprised of the biopolymers contained in the cell walls of plants. The higher order structures of plant cell walls prevent utilization of these carbohydrates due to the "recalcitrance" of lignocellulose, and it is noteworthy that this vast resource of reduced carbon is overwhelming used for its existing structural value (as fiber and as a construction material) or for combustion rather than for the value of its chemical constituents. Increasing adoption of technologies for the production of biobased fuels, chemicals, and materials utilizing plant feedstocks offer one compelling route to achieve these sustainability needs through the capture and redirection of energy and carbon within the carbon cycle. While these products are beginning to enter the market, much of the promise of these technologies has failed to materialize due to commercialization barriers that are both technological and economic. As such, there is a substantial unmet need for both fundamental and applied research in order to achieve these breakthroughs. Our research at Michigan State University has been focused on addressing fundamental and applied problems associated with the conversion of plant-derived biomass to renewable bioproducts through integrated biochemical and chemical catalytic conversion routes (Figure 1).

Unlike the petrochemical refining industry, where processes are designed around feedstock properties, plants can be bred or engineered with phenotypes that are tailored for a desired conversion process. Plants have been bred for millennia to achieve desired phenotypes as food crops, however, research into developing plants with cell walls properties optimized for targeted conversion processes is only beginning and represents an ideal opportunity for collaboration between chemical engineers and plant biologists. The higher order structure of plant cell walls strongly impacts their response to "deconstruction" and conversion. Several recent research projects in the Hodge Laboratory have focused on improving

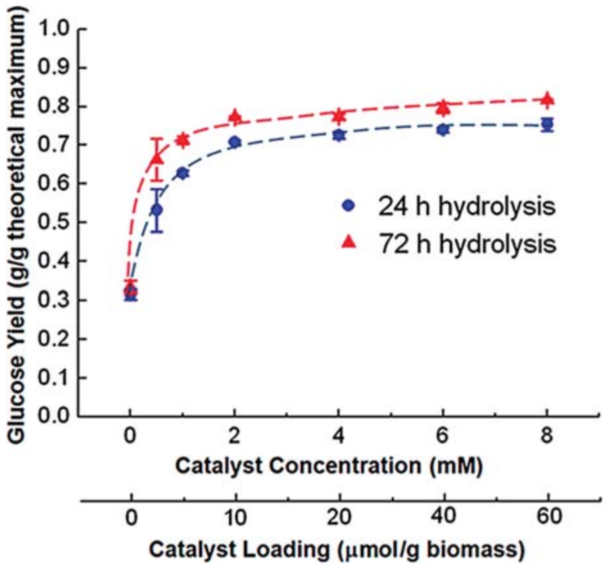

FIGURE 2. Demonstration of improved enzymatic hydrolysis yields using catalyzed oxidative delignification.

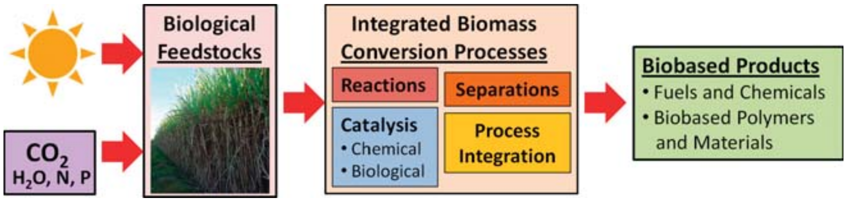

FIGURE 1. Scope of the research program in the Hodge laboratory.

the understanding of how cell wall properties (including higher order structures, hydrophobicity, composition, polymer properties, and cell wall-associated metal content and speciation) contribute to their behavior in conversion processes and how processes can be improved or optimized using this knowledge. In nature, microbes successfully degrade plant cell walls using a variety of oxidative approaches. These strategies include the release of reactive oxygen species produced by redoxactive metals and metalloenzymes. With funding from DOE, we are investigating applying abiotic catalytic oxidative treatments that mimic certain features of these successful biological approaches (Figure 2) that include alkaline-oxidative pretreatment of biomass in the presence of a homogeneous catalyst. Another research theme is cell wall biopolymer extraction, recovery, and catalytic conversion to add value to lignocellulosic biomass conversion processes. This includes research that seeks to understand how the properties of cell wall biopolymers solubilized during alkaline pretreatments or chemical pulping processes impact their processing behavior and how this understanding can be exploited by solubility-based separations processes to extract more value from alkaline pulping or alkaline pretreatment process streams. Building on this, other work is directed at the catalytic conversion of lignins derived from biorefinery and forest products industry process streams to aromatic monomers (Figure 3) as well as understanding the structural features that contribute to lignin reactivity (Figure 4).

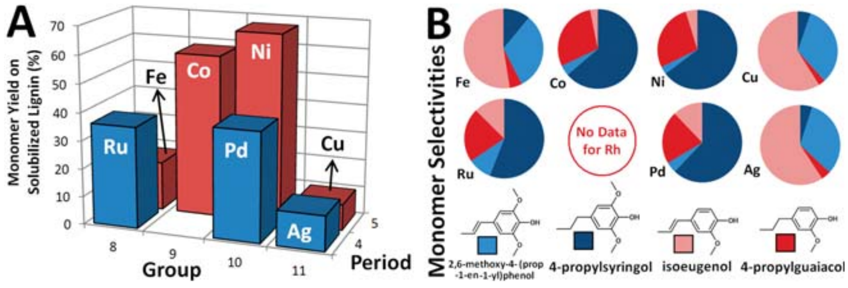

FIGURE 3. Demonstration of (A) high yields and (B) high selectivities for a limited range of monomer products from simultaneous catalyzed delignification and lignin depolymerization of whole birch wood in H-donating solvents without supplemental H_2.

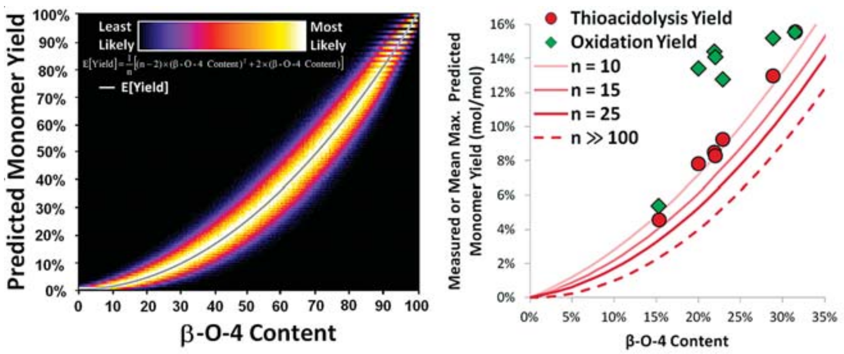

FIGURE 4. Demonstration that yield predictions match experimental yields for C-O cleaving chemical and catalytic lignin depolymerization routes. Simulations are based on random distribution of aryl ethers throughout polymers.

RECENT PUBLICATIONS

N. Bansal, A. Bhalla, S. Pattathil, S.L. Adelman, M.G. Hahn, D.B. Hodge, E.L. Hegg. "Cell wall-associated transition metals improve alkaline oxidative pretreatment in diverse hardwoods," *Green Chem.* (2016). (doi: 10.1039/c5gc01748c)

Z. Li, N. Bansal, A. Azarpira, A. Bhalla, C.H. Chen, J. Ralph, E.L. Hegg, D.B. Hodge. "Chemical and structural changes associated with Cu-catalyzed alkaline-oxidative delignification of hybrid poplar," *Biotechnol Biofuels.* 8, 123 (2015).

M. Li, M. Heckwolf, J.D. Crowe, D.L. Williams, T.D. Magee, S.M. Kaeppler, N. de Leon, D.B. Hodge. "Cell wall properties contributing to alkaline pretreatment and deconstruction of diverse maize (*Zea mays L.*) lines," *J. Exp Bot.* 66(14):4305–4315 (2015).

R.J. Stoklosa, D.B. Hodge. "Fractionation and improved enzymatic deconstruction of hardwoods with alkaline delignification," *Bioenerg Res.* 8(3):1224–1234 (2015).

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T. Liu, D.L. Williams, S. Pattathil, M. Li, M.G. Hahn, D.B. Hodge. "Coupling alkaline pre-extraction with oxidative post-treatment of corn stover to enhance enzymatic hydrolysis and fermentability," *Biotechnol Biofuels.* 7, 48 (2014).

Biorefineries: Integrated Biochemical Processes for Liquid Biofuels, ed. N. Qureshi, D.B. Hodge, A. Vertès. Elsevier Press (2014).

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T.K. Sato, T. Liu, L.S. Parreiras, D.L. Williams, D.J. Wohlbach, B.D. Bice, R.J. Breuer, I.S. Ong, L. Qin, D. Bulsalacchi, S. Deshpande, C. Daum, A.P. Gasch, D.B. Hodge. "Harnessing genetic diversity in saccharomyces cerevisiae for improved fermentation of xylose in hydrolysates of alkaline hydrogen peroxide pretreated biomass," *Appl Env Microbiol*. 80(2):540–554 (2014).

D.L. Williams, D.B. Hodge. ("Impacts of delignification and hot water pretreatment on the water induced cell wall swelling behavior of grasses and its relation to cellulolytic enzyme hydrolysis and binding," *Cellulose*. 21(1):221–235 (2014).

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FIGURE 1. Xinting Lin and Christopher Hershey operating the die-drawing apparatus.

RESEARCH INTERESTS

Polymer composites processing and rheology. Dr. Jayaraman's research interests and expertise are processing, rheology, and microstructure development in polymer composites, polymer nanocomposites, foams, and porous composites, thermoplastic olefin blends (TPO), elastomers, thermoplastic foams and thermoplastic vulcanizate blends (TPV). This research is aimed at developing processing strategies and chemical treatment methods with coupling agents for rheology modification and microstructure development during melt processing and solid-state processing.

WEBSITE

http://www.chems.msu.edu/groups/jay/

SPECIAL EQUIPMENT AVAILABLE

Die-drawing apparatus, TA ARES rheometer with an SER extensional flow fixture for melts and large-amplitude oscillatory shear capability (LAOS), Dynisco capillary rheometer, Polylabs torque rheometer with a Banbury mixer attachment

GROUP MEMBERS

CURRENT PHD STUDENTS: Xinting Lin, Christopher J. Hershey, Xing Lu. RECENT PHD GRADUATES: Amit K. Chaudhary (Dow Chemical Co. Midland, MI), Tanmay J. Pathak (A. Schulman Inc., Akron, OH), Rahul H. Rane (Tata Autocomp Systems, Pune, India), Weijie Ren

CURRENT RESEARCH

High performance additives with nanoparticles for film blowing. Polymer nanocomposites with layered silicates have two different types of interface sites: edges with hydroxyl groups and gallery faces with oxygen atoms. The polymer-particle interface at either site may be strengthened by silane coupling agents. Effects of reactive coupling by the silane and a long chain polymeric compatibilizer at different interface sites have been investigated on the morphology and rheology of polypropylene nanocomposites in the melt-compounded state. The resulting state of dispersion and uniaxial extensional viscosity behavior are shown in the adjacent figure. New masterbatch additives have been developed that may be compounded with bulk polyolefins and used in film blowing to produce films with good tensile strength and tear strength while also having much improved barrier to water vapor.

Die-drawing of microporous polymer composite membranes. High levels of molecular orientation can be produced in semi-crystalline polymers by solid phase processes such as roll-drawing and die-drawing at elevated temperatures below the melting temperature. Die-drawing of particulate filled polyolefins at elevated temperatures was developed recently to produce expanded and oriented particulate composites that are lighter and stronger after processing. The thickness of the sheet produced so far by die-drawing has been 2 mm or more for construction materials. The die-drawing process is now

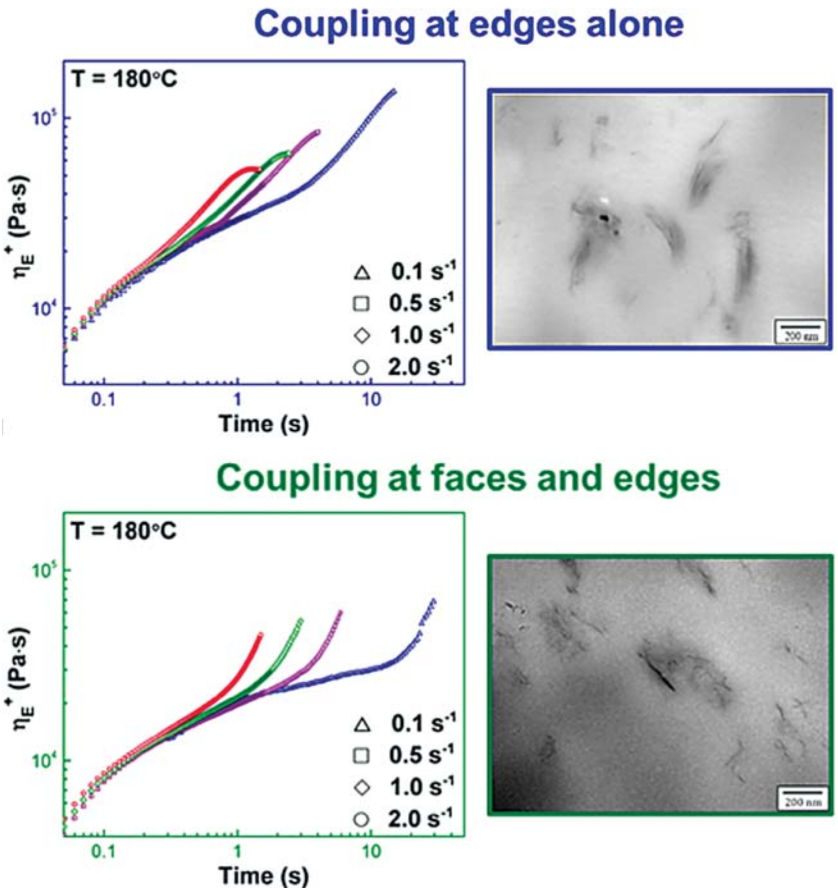
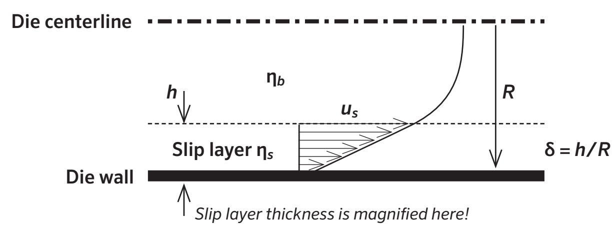


FIGURE 2. Reactive coupling at the interface produces finer dispersions and strain hardening in uniaxial extensional flow of polymer-layered silicate nanocomposites—more so with both coupling at faces and edges.

being applied to produce thinner and stronger porous sheets or membranes: one application area for such membranes is as separators in batteries.

The action of lubricants and other rheology modifiers in polymer compounds. Lubricants can be effective in different ways: (A) by forming a wall layer that is less viscous than the bulk and thus producing apparent slip or (B) by reducing the viscosity of the bulk. The presence of other modifiers such as thickeners or interfacial agents may affect the action of lubricants in the formulation.



This is being studied with polymer composites and thermoplastic elastomer blends. The morphology of the composite or blend is investigated by means of the distribution of sizes and shapes among the disperse particles which may be discontinuous long fibers or elastomer; this is then related to the thickness and viscosity of the slip layer. The slip characteristics are quite sensitive to the presence of interfacial agents added to the compound. This research may be applied specifically to improve the flow during compression molding of discontinuous long fiber filled polymer molding compound.

RECENT PUBLICATIONS

W. Ren, A.K. Chaudhary, K. Jayaraman. "processing polypropylene nanocomposites with silylated organoclays: coupling at edges versus gallery faces," *Ind. Eng. Chem. Res.*, 54, 4264–4273 (2015).

R.H. Rane, K. Jayaraman, K.L. Nichols, T.R. Bieler, M.H. Mazor. "Evolution of crystalline orientation and texture during solid phase die-drawing of PP-talc composites," *J. Polym. Sci., Part B*, 52 (23), 1528–1538 (2014).

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A. B. C. D.

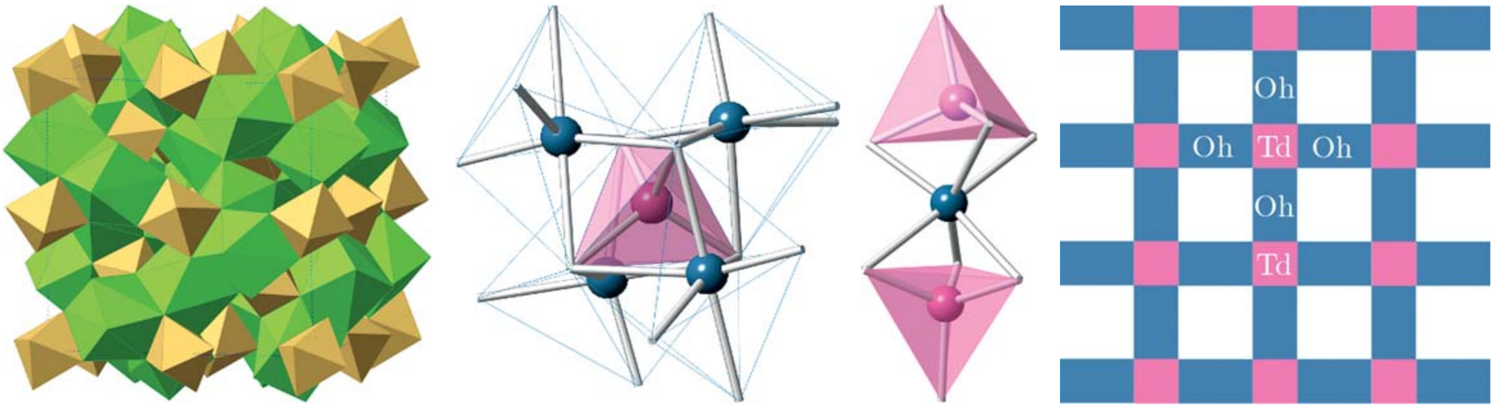


FIGURE 1. (A) La-Ta-O framework, (B) Td-Li, (C) Oh-Li, (D) 2D schematic.

RESEARCH INTERESTS

Advanced materials and electroanalytical methods for energy conversion and storage technologies

LAB

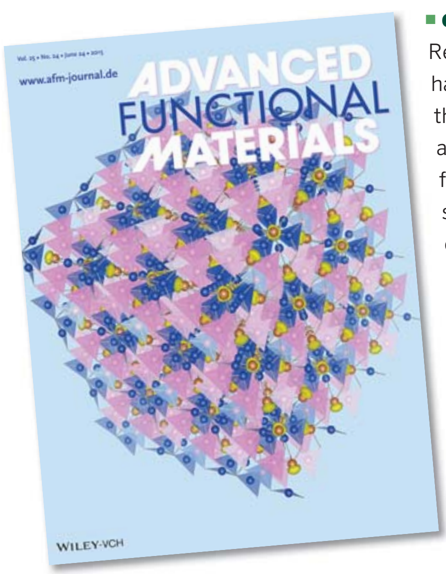
Advanced Energy Materials Lab

WEBSITE

http://weilaigroup.org

GROUP MEMBERS

GRADUATE STUDENTS: Matt Klenk, Junchao Li, Qian Chen, Jin Dai. CO-ADVISED GRADUATE STUDENTS: Tobias Glossmann (Oakland University). UNDERGRADS: Yalun Cai, Sydney Boeberitz, Dong Feng



CURRENT RESEARCH

Research interests in our lab have been broadly focused on the study of advanced materials and electroanalytical methods for energy conversion and storage technologies. Recently our research effort has centered around Solid-state Ionic Conductors (SIC) and Solid-state Mixed Ionic and Electronic Conductors (SMIEC) as battery electrolytes/ electrodes and thermoelectric (TE) materials. SIC, SMIEC, and TE compounds are all complex materials with a framework-guest structure and unique ionic and electronic properties. The guest atoms in SIC and SMIEC are able to diffuse or conduct, while the framework is insulating (SIC) or semiconducting (SMIEC) for electrons, respectively. The guest atoms in TE are rattlers while the framework is semiconducting for electrons. The complexity of these materials calls for techniques known to both crystallographers and non-crystallographers. We are applying a suite of average and local structure and dynamics probes to understand their fundamental structure-property relationships.

Ongoing projects include:

Structure and dynamics of lithium-stuffed garnet oxides. State-of-the-art Li-ion batteries utilize organic solvent based liquid electrolytes that usually have limited electrochemical stability and are also volatile and flammable. Lithium-stuffed garnet oxides are a new class of nonflammable solid electrolytes with high lithium ionic conductivities. The framework of the materials is composed of LaO_8 dodecahedra and TaO_6 octahedra. There are two types of cages, tetrahedral (Td) and octahedral (Oh), to host lithium ions. Each Td cage is surrounded by four Oh cages and each Oh cage is surrounded bytwo Td cages. Both the Td and Oh cages are only partially occupied. We are investigating a prototypic series of lithium-stuffed garnet oxides $Li_{7-x}La_3Zr_{2-x}Ta_xO_{12}$ (x = 0–2). The scientific goal is to understand structure and dynamics of lithium disorder in these complex materials. FUNDING: National Science Foundation.

Structure and dynamics of thermoelectric materials. Currently around two-thirds of energy produced in US is rejected mainly in the form of waste heat. Such unused heat can be recovered by thermoelectric processes that directly convert thermal

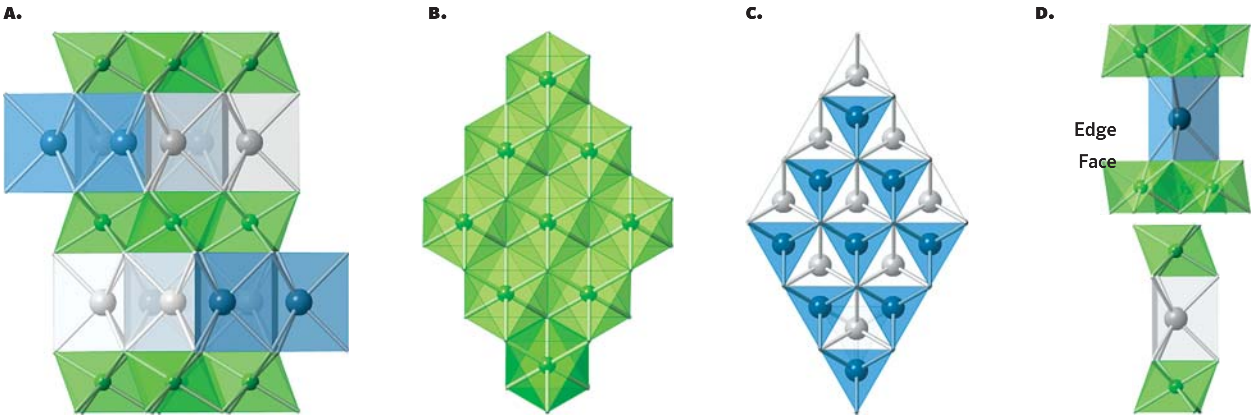


FIGURE 2. (A) $Na_{2x}(Ni_xTi_{1-x})O_2$, (B) $[(Ni^{2+}, Ti^{4+})O_2]$: electronic, (C) Na^eO_6 and Na^fO_6: ionic, (D) ionic-electronic interaction.

energy into electricity. Robust and cost-effective thermoelectric devices could have significant impact on the energy production and utilization of the society. Tetrahedrites are a class of TE materials based on $Cu_{12}Sb_4S_{13}$ containing earth-abundant and environmentally friendly elements. The structure consists of a 3D framework of CuS_4 tetrahedra and SbS_3 polyhedra. Another type of Cu atoms (Cu12e) behave as rattling guests inside a cage formed by three S and two Sb atoms. The interaction between Cu12e and Sb atoms is mitigated by the Sb lone pairs. We are currently investigating the relationship between atomic and electronic structure and thermoelectric properties of undoped and doped $Cu_{12}Sb_4S_{13}$ tetrahedrites. FUNDING: National Science Foundation (in collaboration with Donald Morelli).

"Bi-functional" electrode materials for Na-ion batteries. While Li-ion batteries have dominated the portable electronics market and started their penetration into the transportation and stationary markets, there is growing concern over the lithium abundance and geographical constraints of lithium minerals. Sodium element is more than 1000 times more abundant than lithium in earth's crust and sea and sodium resources are considered practically unlimited. We are studying a class of sodium mixed oxides, $Na_{2x}(Ni_xTi_{1-x})O_2$, that have both high redox-potential transition metals, e.g. Ni, and low redox-potential transition metals, e.g., Ti. This suggests that these materials can be either utilized as a cathode or an anode, i.e., "bi-functional." FUNDING: National Science Foundation.

RECENT PUBLICATIONS

J.C. Li, M.Z. Zhu, D.L. Abernathy, X.L. Ke, D.T. Morelli, W. Lai, "First-principles studies of atomic dynamics in tetrahedrite thermoelectrics," *APL Mater.*, 4, 104811 (2016).

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M. Klenk, W. Lai, "Local structure and dynamics of lithium garnet ionic conductors: tetragonal and cubic $Li_7La_3Zr_2O_{12}$," *Phys. Chem. Chem. Phys.*, 17, 8758 (2015).

Y. Wang, W. Lai, "Phase transition in lithium garnet oxide ionic conductors $Li_7La_3Zr_2O_{12}$: The role of Ta substitution and H_2O/CO_2 exposure," *J. Power Sources*, 275, 612 (2015).

R. Shanmugam, W. Lai, "Study of transport properties and interfacial kinetics of $Na_{2/3}[Ni_{1/3}Mn_xTi_{2/3-x}]O_2$ ($x = 0, 1/3$) as electrodes for Na-ion batteries," *J. Electrochem. Soc.*, 162, A8 (2015).

Andre Lee

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RESEARCH INTERESTS

Electronic packaging materials, solidification of materials, high-temperature polymers and their composites, phase, and synchrotron characterization

LAB

Inorganic-Organic Synthesis and Processing (3545 Engineering Bldg.)

SPECIAL EQUIPMENT AVAILABLE

Confocal Raman spectrometer with environmental control deformation chamber, high-pressure differential scanning calorimeter, rheometer, dynamic solid analyzer

GROUP MEMBERS

UNDERGRADUATE STUDENTS: Eric Egedy, Risa Hocking.
PHD STUDENTS: Yang Lu, Yueline Wu, David Vogelsang.
COLLABORATING FACULTY: Prof. Robert Maleczka (Chemistry).

PATENTS

"Nanostructured chemicals as alloying agents in polymers," A. Lee, J.D. Lichtenhan, J.J. Schwab, S.H. Phillips. US Patent No. 6716919 (2004).

"High use temperature nanocomposite resins," A. Lee, J.D. Lichtenhan, Q. Liu, X. Fu, S. Hait, J.J. Schwab, R.L. Blanski, P.N. Ruth. US Patent 7553904 (2009).

"Composite metal matrix castings and solder compositions, and methods," A. Lee, K.N. Subramanian. US Patent 7572343 (2009).

CURRENT RESEARCH

Electrochemical behavior of Cu-Al intermetallics in Cu wire bonding packages. Wire bonding is a key packaging technology to achieve the electrical and mechanical interconnections between integrated circuit and the metal frame in printed circuit board. Recently, copper (Cu) has gained popularity over gold (Au) as the wire material based on cost reduction and higher performance. Two major intermetallics (IMCs), θ ($CuAl_2$) and γ (Cu_9Al_4), are often found in the Cu-Al bonding interface after the as-bonded structure undergoes thermal aging for extended periods of time. Galvanic corrosion for this Cu/γ/θ/Al metallic-intermetallic "sandwich" structure, may take place when dissimilar metals are brought into electrical contact in the presence of an electrolyte containing corrosive species. In the service environment, moisture absorbed by the molding compound can dissolve a small amount of halogens (Cl^-, Br^-) used in the synthesis of molding compound and act as the electrolyte to initiate galvanic corrosion. Several studies have reported that the mechanical failure resulted from the disappearance of γ and failure occurred at the wire side. The use of Pd-coated Cu wire had shown to enhanced service reliability. It was suggested that the enhanced service reliability maybe due to the nobility of Pd addition, however, no systematic electrochemical characterization has been carried out for each of the entities in Cu(Pd)-Al bonding interface, which is essential to understand corrosion behavior of Cu(Pd)-Al bonding interface.

Using open circuit potentials and potentiodynamic polarization measurements systemic investigate were performed on all the undoped/Pd-doped samples (Cu, γ, θ) in different pH, Cl^- concentration and temperatures to provide a complete picture of electrochemical behavior needed to understand the service reliability of wire boned electronic packages. Electrochemical characteristic of metals were examined using cathodic and anodic polarization curves. Both E_{corr} and i_{corr} are determined by the thermodynamics (reversible potentials: $E(M/M^{n+})$, $E(O_2/OH^-)$) and kinetics (exchange current densities: $i_0(M/M^{n+})$, $i_0(O_2/OH^-)$, Tafel constants) of the two half-cell reactions. The addition of Pd increases the cathodic current density by increasing the exchange current density for ORR, and reduces the anodic current density by the induced passivation. This upward shift on the cathodic polarization curve, as well as the downward shift on the anodic polarization curve, led to an increase in the value of E_{corr}. However, the change in the value of i_{corr} depends on the relative amount of shift between cathodic and anodic polarization curves. As shown in Figure 1(a), the upward shift in the cathodic polarization curve was more than the downward shift in the anodic polarization, the value of icorr will increase, which meaning a faster rate of corrosion. This was the case when only small amounts of Pd addition in Cu. To reduce the value of i_{corr}, it was necessary that the amount of downward shift be greater than the amount of upward shift, Figure 1(b). Therefore, a higher amount of Pd was needed to reduce the corrosion rate.

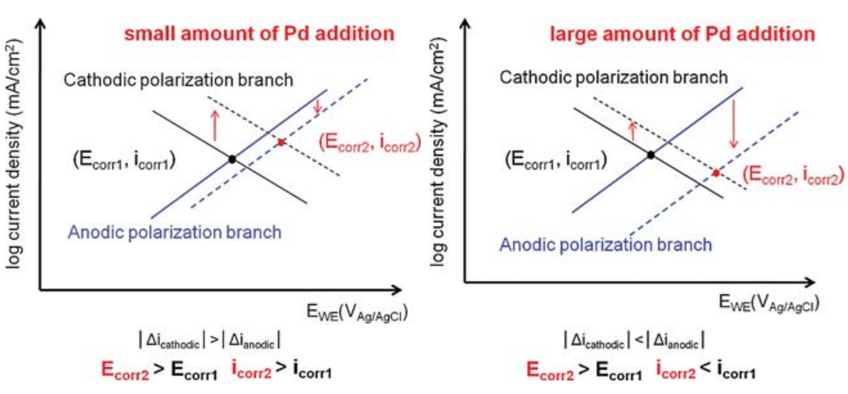

FIGURE 1. Determination of E_{corr} and i_{corr} of *g* using polarization curves. The addition of Pd causing an upward shift of the cathodic branch and a downward shift of anodic branch of the polarization curve, leading to changes in E_{corr} and i_{corr}.

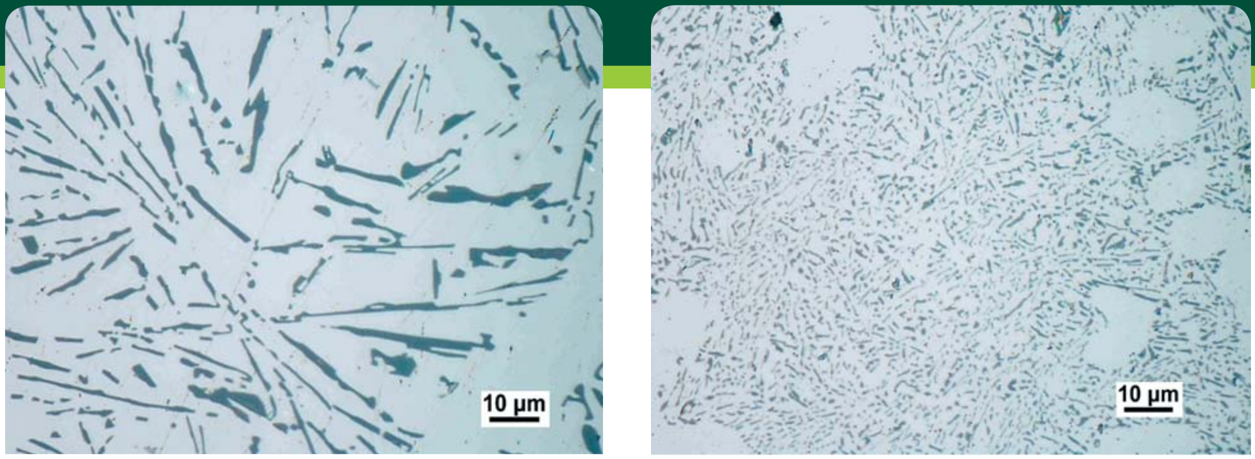

FIGURE 2. Optical micrograph of an ingot made of A4047 powders (*left*) without POSS trisilanol and (*right*) with POSS trisilanol.

Influence of nano-structured silanols on the microstructure of Al-Si casting alloys. Aluminum (Al) based casting alloys have been used as light-weighting materials in the automotive industry for decades. Further weight reduction has been introduced in the automotive body construction recently with the use of structural aluminum. However, without modification, most of Al casting alloys have poor ductility, and does not meet the structural application requirement, i.e., at least 12% elongation to failure. Although, the addition of Na or Sr can spheroidize Si cuboids, and the addition of Ti and B reduce the grain size of primary aluminum phase in Al-Si based casting alloys. However, these modifications had some drawbacks needed to overcome, such as coarsening with aging as well as fading with repeated melting. Polyhedral oligomeric silsequioxanes (POSS) are silsequioxane-based nano-structural chemicals. These chemicals are cage like structures with repeated monomer units of $RSiO_{1.5}$ where Si is the element silicon, O is oxygen and R is hydrocarbon group, e.g., ethyl, isobutyl, phenyl etc. Partial cage-like POSS have the thermal stability in the molten aluminum and the silanol (Si-OH) functionalities form thermodynamically stable Si-O-M bonds with metals (e.g., Al). These nano-sized silanol compounds provide nucleation sites during solidification as grain refiner, and also serve as obstacles for preventing coarsening at elevated temperatures for microstructural stability of Al alloys.

A4047 and A4047 powders with and without POSS trisilanol added were used to make ingots for metallographic study. Figure 2 shows the optical micrographs of the ingots made of 325 mesh A4047 powders without and with POSS trisilanol addition, respectively. A4047 has a near-eutectic Al-Si composition with primary Al phase and eutectic Si-Al phase. Figure 2 (*left*) displays the microstructure of A4047 without POSS trisilanol, which is typical from a slow-cooled ingot with Al dendrite and lamellar Si cuboids. With the addition of POSS trisilanol, under the same casting and cooling configurations, the Si platelets are broken down to very fine spheroidized phase, as shown in Figure 2 (*right*).

The microstructure modification with POSS trisilanol added also leads to significant benefit in the mechanical property of A4047. Tensile tests were conducted on the tensile bars machined from the ingots. It was found that the elongation to failure had increased with POSS trisilanol addition, with percentage increase from 23% to 250% over the control sample (without POSS trisilanol added). In addition, the ultimate tensile strength did not decrease with the benefit of increases in the elongation to failure. Currently we are exploring different approaches for produce master alloys with different Si contents from hypoeutectic to hypereutectic Al-Si casting alloys.

RECENT PUBLICATIONS

Y. Zho, L. Ma, F. Guo, L. Qiao, Y. Shu, A. Lee, K.N. Subramanian. "Effects of electromigration on the creep and thermal fatigue behavior of $Sn_{58}Bi$ solder joints," *J. of Electronic. Mat.*, 43, 4395 (2014).

B.W. Schoen, C.T. Lira, A. Lee. "Separation and solubility of *cis* and *trans* isomers in nanostructured double-decker silsesquioxane," *J. of Chem. and Eng. Data*, 59, 1483 (2014).

S. Liu, L. Ma, Y. Shu, K.N. Subramanian, A. Lee, F. Guo. "Effects of POSS-silanol addition on whisker formation in Sn-based Pb-free electronic solders," *J. of Electronic. Mat.*, 43, 26 (2014).

B.W. Schoen, D. Holmes, A. Lee. "Identification and quantification of cis and trans isomers in aninophenyl double-decker silsesquioxanes using 1H-29Si gHMBC NMR," *Magn. Reson. in Chem.*, 51, 490 (2013).

A. Lee, D. Choudhuri, K.N. Subramanian. "Effect of temperature-dependent deformation on TMF reliability of eutectic Sn-Ag solder joints," in *Lead-Free Solders: Materials Reliability for Electronics*, Wiley (2012).

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RESEARCH INTERESTS

Nanotechnology, polymers, adhesion, particles, biomimetics, self-assembly, nanomixing, nanodispersion, separation, renewable bioenergy, fluid flow

LAB

Polymer Surface, Interface, Nanotechnology Research Group (2522 Engineering Bldg.)

WEBSITE

http://www.egr.msu.edu/~leeil/

SPECIAL EQUIPMENT AVAILABLE

Brookheaven ZetaPALS dynamic light scattering particle size analyzer/zeta potential analyzer; Primix TK Filmix ultra high-speed, thin-film mixer designed to produce stable nanodispersions; fluorescent and phase contrast optical micrographs with a digital camera connected to a computer (Nikon Eclipse ME 600 and ME 400 microscopes); layer-by-layer assembly and microcontact printing facilities; programmable slide stainer (Zeiss), spin coater, centrifuge, plasma cleaner (Harrick)

GROUP MEMBERS

Jing Yu, Anna Song, Dr. Joung Sook Hong, Brooke Meharg, Chris Tawfik

PATENTS

"Micropatterning of conductive graphite particles using microcontact printing," I. Lee, L.T. Drzal, J. Lu, T.R. Hendricks. US Patent 9,023,47 (5/5/2015).

"One-step method for pretreating biomass using nanomixing," I.Lee, W. Wang, S. Ji. US Patent 8,741,632 (6/3/2014).

RECENT ACHIEVEMENTS

The poster "Development of Layered Multi-scale Porous Thin Films by Tuning Deposition Time and Molecular Weight of Polyelectrolytes" by J. Yu, O. Sanyal, A.P. Izbicki, I. Lee won the First-Place Poster Award ($500) in the Materials Science and Engineering Division (MSED) at the AIChE 2015 Annual Meeting in Salt Lake City, UT (November 8–13, 2015)

Affordable production of cellulose nanowhiskers (MIIE); Solar-Bio-Nano Based Wastewater System for the Production of Energy and Potable Water (DOD- SERDP); Understanding and Modulation of Electrostatic and Hydrophobic Forces within; Plant Cell Walls to Facilitate Enzymatic Deconstruction and Conversion to Biofuels (NSF); Prevention of Bacterial Biofilm Formation on Surfaces (SPG)

CURRENT RESEARCH

Dr. Ilsoon Lee's nano bio engineering laboratory is utilizing nanotechnology and self-assembly as new tools to design new nanostructured materials and systems to solve existing engineering problems in energy, materials, and environment. The research focuses on the design and fabrication of nano / bio particles and films to advance energy, biocatalytic systems, and functional materials.

Specific selective projects include:

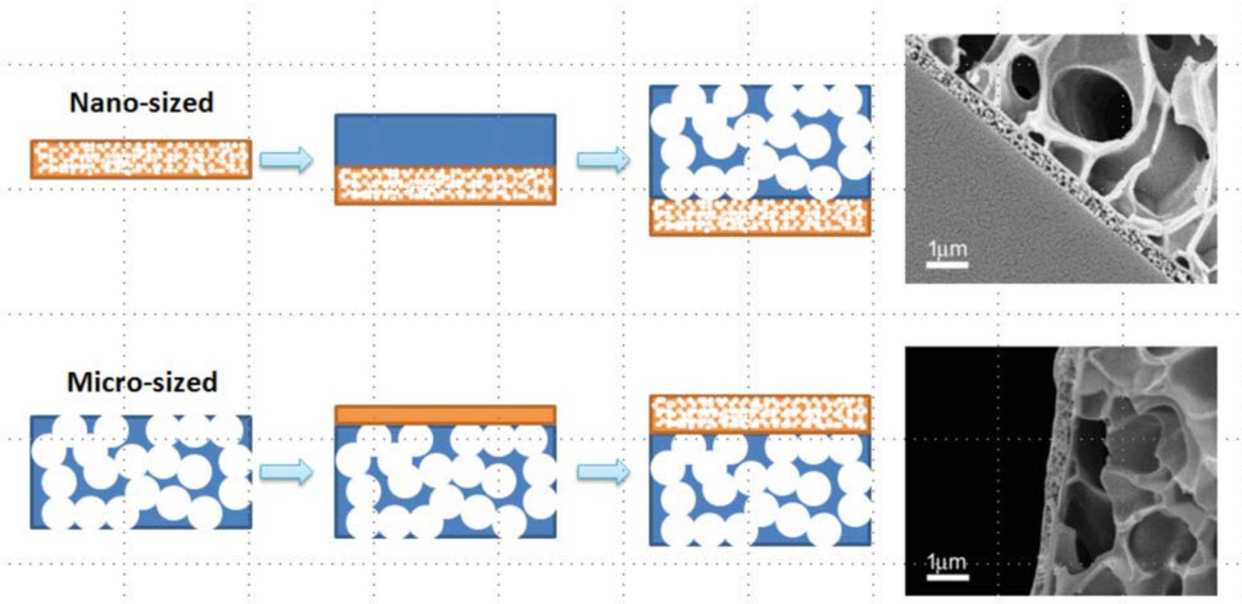

FIGURE 1. This work focuses on the design of porous polymeric films with nano- and micro-sized pores existing in distinct zones.

- Prevention of bacterial biofilm formation on surfaces
- Solar-bio-nano based wastewater system for the production of energy and potable water
- Hybrid nanostructured metal foam material systems for blast impact (and wrinkle-free films)
- Fabrication of functional nanoparticles and delivery system
- Fast and efficient production of cellulose nanowhiskers and the use in the composite materials
- Understanding and modulation of interfacial properties within plant cell wall pores to facilitate enzymatic deconstruction and conversion to biofuels.

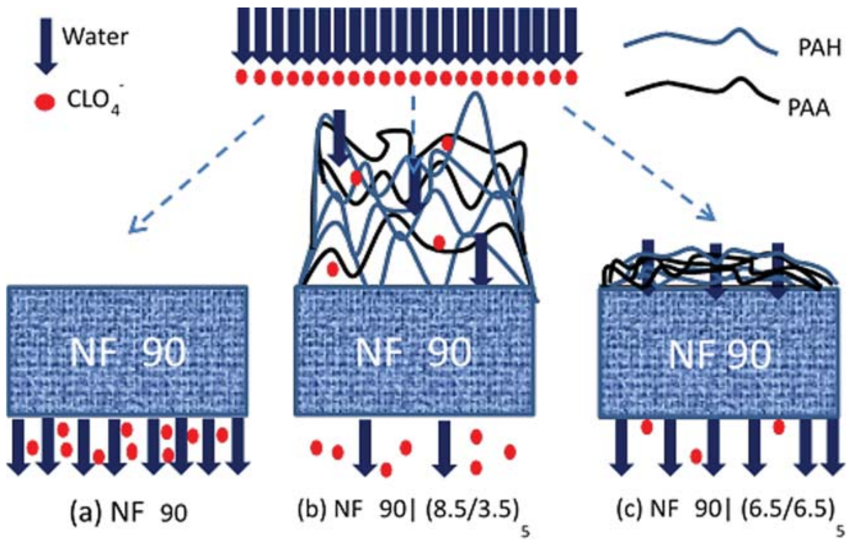

FIGURE 2. Perchlorate rejection enhanced by surface modification via LbL assembly technique. Optimized membrane had much higher permeability and equivalent rejection than RO.

FIGURE 3. Surfaces and interfaces capable of repelling, attracting, and selectively detecting molecules have attracted attention for their important application in catalysts, coatings, sensors, and devices, including biologically implantable ones.

RECENT PUBLICATIONS

O. Sanyal, Z. Liu, B.M. Meharg, W. Liao, I. Lee. “Development of polyelectrolyte multilayer membranes to reduce the COD level of electrocoagulation treated high-strength wastewater,” *Journal of Membrane Science* 496, 259–266 (2015).

J. Yu, O. Sanyal, A.P. Izbicki, I. Lee. “Development of layered multi-scale porous thin films by tuning deposition time and molecular weight of polyelectrolytes,” *Macromolecular Rapid Communications* 36, 1669–1674 (2015).

O. Sanyal, O.; Sommerfeld, A.N.; Lee, I. “Design of ultrathin nanostructured polyelectrolyte-based membranes with high perchlorate rejection and high permeability,” *Separation and Purification Technology* 145, 113–119 (2015).

A.A. Gokhale, J. Lu, R.R. Weerasiri, J. Yu, I. Lee. “Amperometric detection and quantification of nitrate ions using a highly sensitive nanostructured membrane electrocodeposited biosensor array,” *Electroanalysis* 27, 1127–1137 (2015).

Y. Sun, R. Burgueño, W. Wang, I. Lee. “Modeling and simulation of the quasi-static compressive behavior of Al/Cu hybrid open-cell foams,” *International Journal of Solids and Structures* 54, 135–146 (2015).

O. Sanyal, I. Lee. “Recent progress in the applications of layer-by-layer assembly to the preparation of nanostructured ion-rejecting water purification membranes,” *Journal of Nanoscience and Nanotechnology* 14, 2178–2189 (2014).

Y. Sun, R. Burgueño, W. Wang, I. Lee. “Effect of annealing on the mechanical properties of nanocopper reinforced open-cell aluminum foams,” *Materials Science and Engineering A* 613, 340–351 (2014).

S. Ji, J. Lu, Z. Liu, D. Srivastava, A. Song, Y. Liu, I. Lee. “Dynamic encapsulation of hydrophilic nisin in hydrophobic poly (lactic acid) particles with controlled morphology by a single emulsion process,” *Journal of Colloid and Interface Science* 423, 85–93 (2014).

A. Peyvandi, S.U. Abideen, Y. Huang, I. Lee, P. Soroushian, J. Lu. “Surface treatment of polymer microfibrillar structures for improved surface wettability and adhesion,” *Applied Surface Science* 289, 586–591 (2014).

Y. Sun, R. Burgueño, A.J. Vanderklok, S.A. Tekalur, W. Wang, I. Lee. “Compressive behavior of aluminum/copper hybrid foams under high strain rate loading,” *Materials Science and Engineering A* 592, 111–120 (2014).

A.A. Gokhale, I. Lee. “Recent advances in the fabrication of nanostructured barrier films,” *Journal of Nanoscience and Nanotechnology* 14, 2157–2177 (2014).

Carl Lira

Associate Professor
lira@egr.msu.edu | 517.355.9731 | 428 S. Shaw Lane, Room 2261

RESEARCH INTERESTS

Properties of bio-derived chemicals and fuels

LABS & LOCATIONS

Properties Lab, 418 S. Shaw Lane, Room 2255.
Reactive Distillation Pilot Facility, 3900 Collins Rd.

WEBSITES

http://researchgroups.msu.edu/liragroup
http://researchgroups.msu.edu/reactivedist

SPECIAL EQUIPMENT AVAILABLE

Vapor-liquid equilibria measurements, flash point, cloud point, densitometry, low- and high-pressure speed of sound

GROUP MEMBERS

Aseel Bala-Ahmed, Dr. Lars Peereboom

RECENT PATENTS

""Integrated Process of Distillation with Side Reactors for Synthesis of Organic Acid Esters," C.B. Panchal, J.C. Prindle, A. Kolah, D.J. Miller, C.T. Lira. US Patent 9174920 B1 (11/3/2015).

"Methods for making 1,3-dihydroxyacetone (DHA) from glycerol," D.J. Miller, X. Hong, C.T. Lira, O. McGiveron. US Patent 8,735,633 B2 (5/27/2014).

CURRENT RESEARCH FOCUS

Make it, boil it, dissolve it, purify it. The Lira Research group is fascinated by characterizing these relatively common properties for pure components and mixtures, and the way the chemical structure determines these properties. When an alternative fuel is developed and blended with petroleum fuel, what are the cold flow properties? What is the effect on the boiling curve? When new chemicals are made from renewable feedstocks, how will they behave in a reactive distillation column? We are also interested in improving modeling of vapor-liquid-liquid equilibria that occurs frequently for bioderived molecules.

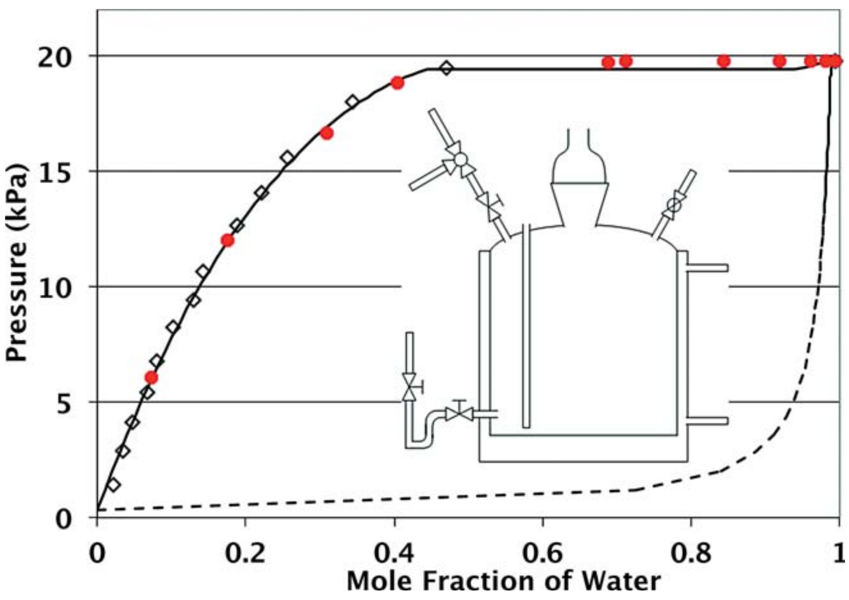

FIGURE 1. P-x diagram of ethyl levulinate + water at 60°C compared with the NRTL-HOC model.

Phase equilibria measurements. The Lira Thermodynamics Research Facility measures and correlates vapor-liquid equilibria (VLE), liquid-liquid equilibria (LLE), solid-liquid equilibria. For VLE, the lab has a Fisher T-xy recirculating apparatus, a custom P-xy apparatus, and a miniature ebuilliometer. We also have capabilities for density and viscosity measurements.

Our phase equilibria measurements support the MSU reactive distillation facility and were vital in development of our process development for diethyl succinate by reactive distillation. We have filed a patent on a process to react the sodium succinate salt directly from the fermentation product to diethyl succinate intermediates, bypassing isolation of succinic acid. An example of P-x measurements are shown in Figure 1, for ethyl levulinate + water. RECENT SPONSORS: DOE, DLA, misc industry. COLLABORATORS: Dennis Miller

Alternative fuel properties. This work models properties of alternative fuels and their blends with petroleum-derived fuels. Differing fuel properties can create compatibility issues in the field. We are developing methods to quickly characterize the behavior of blends and provide predictive tools for blend cloud point, distillation curve, average molecular weight and cetane number. Surrogates with a finite number of components are used to represent the paraffin, isoparaffin, aromatic, and naphthene distribution in the fuels. Alternative fuels have composition profiles significantly different than petroleum fuels. Figure 2 shows the distillation curve behavior of traditional JP-8 fuel and several alternative fuels. SPONSORS: US Army, Tank Automotive Research Development and Engineering Center. COLLABORATORS: Eric Sattler (USA), Nicole Hubble (USA), Linda Schafer (USAF).

Improved association-based models for separations in the bioeconomy. With industrial focus moving to bioderived feedstocks, the need for improved process modeling is acute; conventional models with adjustable parameters do not correlate data accurately enough for extrapolations in temperature or to new compositions. Thus, precise process design for streams with these components requires many experimental measurements and expensive, slow pilot-plant

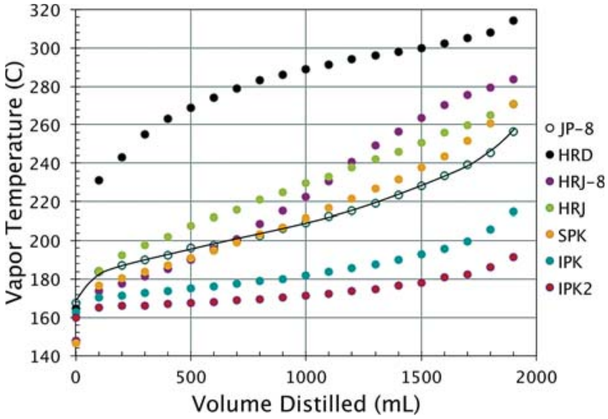

FIGURE 2. Fuel volatility is related to both ease of starting. Note the wide distribution of boiling behavior exhibited by the fuels.

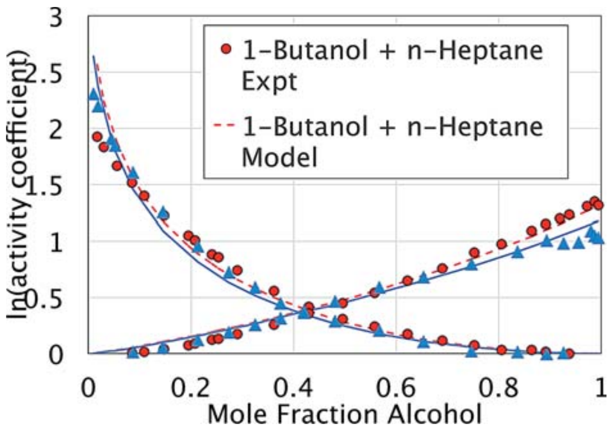

FIGURE 3. After representing the hydrogen bonding in pure alcohols, the predictions of solution nonidealities in mixtures with hydrocarbons are well captured without using any adjustable mixture parameters.

studies. Improved models will greatly enhance the efficiency of renewables-based process development. This project is developing improved models that include meaningful representation of hydrogen bonding of oxygen-containing molecules. Popular predictive and correlative models (UNIFAC, NRTL) do not use the correct functional form to represent hydrogen bonding. This work strives to integrate association approaches such as Wertheim's theory together with meaningful spectroscopic measurements and quantum chemical calculations to improve modeling of hydrogen-bonding system. Figure 3 shows an early version of the modeling capabilities. COLLABORATORS: James (Ned) Jackson (Chemistry), N. Patel (Dow Chemical), P. Mathias (Fluor), T. Frank and D. Vu (Dow Chemical), and E. Cheluget (Honeywell).

RECENT PUBLICATIONS

A.L. Lown, L. Peereboom, J. van Shaik, C.T. Lira. "Cetane numbers and compressibility of JP-8/biofuel blends," Final Report, U.S. Army TARDEC Contract W56HZV-13-C-0340, 256 pp. (10/19/2015).

F. Leyva, A. Orjuela, A. Kolah, C. Lira, D. Miller, G. Rodríguez. "Isoamyl propionate production by reactive distillation," *Separation and Purification Technology* 146, 199 (2015).

T.L. Jordison, C.T. Lira, D.J. Miller. "Condensed-phase ethanol conversion to higher alcohols," *Ind. Eng. Chem. Res.* 2015, 54 (44), 10991.

B.W. Schoen, C.T. Lira, A. Lee. "Separation and solubility of cis and trans isomers in nanostructured double-decker silsequioxanes.," *Journal of Chemical and Engineering Data* 59, 1483–1493 (2014). (doi: 10.1021/je4010245)

A.J. Resk, L. Peereboom, A.K. Kolah, D.J. Miller, C.T. Lira. "Phase equilibria in systems with levulinic acid and ethyl levulinate," *Journal of Chemical and Engineering Data* 59, 1062–1068 (2014). (doi: 10.1021%2Fje400814n)

A.L. Lown, L. Peereboom, S.A. Mueller, J.E. Anderson, D.J. Miller, C.T. Lira. "Cold flow properties for blends of biofuels with diesel and jet fuels," *Fuel*, 117PA, 544–551 (2014). (doi: 10.1016/j.fuel.2013.09.067)

D.J. Miller, A.K. Kolah, C.T. Lira. "Reactive Distillation for the Biorefinery," Chapter 20, in *Separation and Purification Technologies in Biorefineries*; H.J. Huang and S. Ramaswamy, eds., New York, J.W. Wiley and Sons (2013).

A. Orjuela, C.T. Lira, D.J. Miller. "A novel process for recovery of fermentation-derived succinic acid: Process design and economic analysis," *Bioresource Technology*, 139, 235–241 (2013). (doi: 10.1016/j.biortech.2013.03.174)

X. Hong, O. McGiveron, A.K. Kolah, A. Orjuela, L. Peereboom, C.T. Lira, D.J. Miller. "Reaction Kinetics of glycerol acetal formation via transacetalization with 1,1-diethoxyethane," *Chemical Engineering Journal*, 222, 374–381 (2013). (doi: 10.1016/j.cej.2013.02.023)

A. Santhanakrishnan, A. Shannon, L. Peereboom, C.T. Lira, D.J. Miller. "Kinetics of mixed ethanol/n-butanol esterification of butyric acid with Amberlyst 70 and p-toluene sulfonic acid," *Ind. & Eng. Chem. Res.*, 52, 1845–1853 (2013). (doi: 10.1021/ie302267s)

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RESEARCH INTERESTS

Organic and molecular electronics, quantum dots, renewable energy, solar cells, light-emitting diodes, excitonic photophysics, crystal growth, molecular therapeutics and imaging

LAB

Molecular and Organic Excitonics Laboratory

WEBSITE

http://www.egr.msu.edu/~rlunt/

SPECIAL EQUIPMENT AVAILABLE

Thin film device fabrication, patterning, and testing; in-situ diffraction; ellipsometry; luminescence spectroscopy

GROUP MEMBERS

POSTDOCS: Dianyi Liu, Lily Wang. GRADUATE STUDENTS: Matthew Bates, Pei Chen, Padmanaban (Paddy) Kuttipillai, Alex Renny, Chris Traverse, Chenchen Yang, Margaret (Peggy) Young. UNDERGRADS: Kevin Chase, Mark Elinski, Audrey Guest, Lucas Layher, Nathan Maise, Tyler Patrick, Adam Redoute, Brian Wingate.

RECENT PATENTS

"Nanocluster light emitting diodes," R.R. Lunt, P. Kuttipillai. US Patent 9,331,298, (5/2016).

"Light trapping architecture for photovoltaic and photodetector applications," S.R. Forrest, R.R. Lunt, M. Slootsky. US Patent 9,412,960 (8/9/2016).

"Transparent photovoltaic cells," R.R. Lunt, V. Bulovic. Patent issued RU 2016, MX 2016.

RECENT ACHIEVEMENTS

Johansen Crosby Endowed Chair (2016)
Withrow Distinguished Junior Scholar Award (2016)
MSU Teacher Scholar Award (2016)
Top Innovators Under 35 List, *Technology Review* (2015)
Ovshinsky Sustainable Energy Fellowship Award, American Physical Society (APS) (2015)
MSU Undergraduate Research Faculty Mentor of the Year Award (2015)
MSU Innovation of the Year Award (2015)
Camille and Henry Dreyfus Postdoctoral Environmental Chemistry Mentor Award (2015)
DuPont Young Professor Award (2013)
NSF CAREER Award (2013)

CURRENT RESEARCH

The Molecular and Organic Excitonics laboratory focuses on inorganic and organic excitonic materials for (1) low-cost solar energy production and (2) efficient energy utilization. We aim to synthesize and exploit oriented, crystalline, nanostructured, and excitonic thin film semiconductors through organic-inorganic and organic-organic interactions while studying fundamental relationships between growth, structure, and photophysical properties. We look to apply this understanding to enhance device performance and create unique electronic functionality.

Routes to lower cost solar cells through nanostructured and excitonic materials. The Earth is continuously bathing in over one-hundred-million-billion watts of sunlight—several thousand times more than mankind's energy demands. While a multifaceted approach is required to transition away from fossil fuels, solar energy will surely be key to a sustainable future. The engineering of PV structures at the nanoscale has attracted research interest as it may enable substantial reductions in PV installation costs and facilitate wider market penetration. Ultimately we aim to further evaluate and exploit these new materials in thin-film architectures to realize ubiquitous and low-cost solar energy.

Excitonics for building integrated transparent PVS and solar concentrators. We are pioneering transparent molecular photovoltaics that can retain a high degree of visible-transparency, while absorbing ultraviolet and near-infrared light for power generation. These cells can allow for optimization of overall transparency, efficiency, and lighting aesthetic and

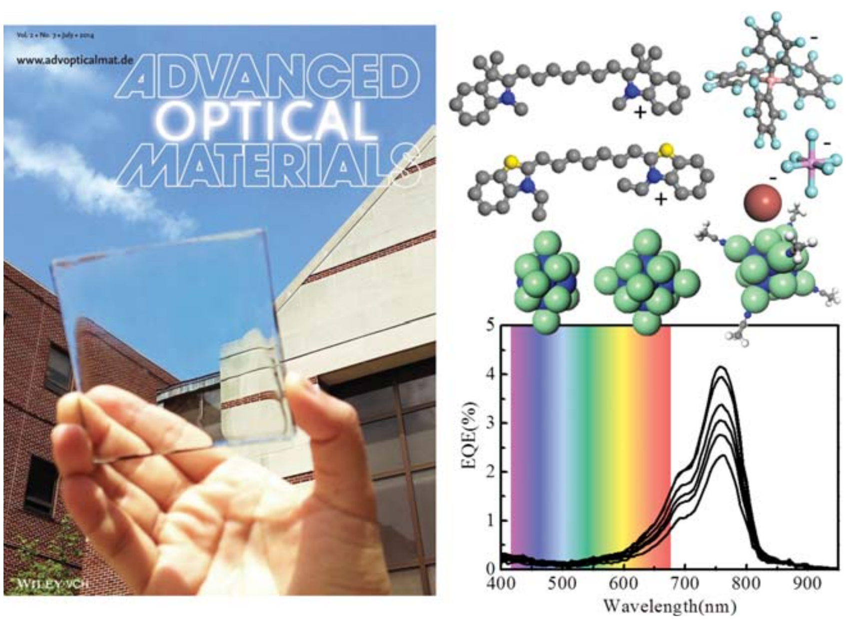

FIGURE 1. LEFT: Highlight of our work on the cover of *Adv Optical Materials* showing a photograph of the pioneering transparent luminescent solar concentrator (LSC) system that selectively harvests infrared light. RIGHT: Diagram of excitonic molecules for these transparent concentrators (*top*) and the demonstrated quantum efficiency in the infrared (*bottom*).

lead to a highly deployable solar window that is retrofittable in window panes in homes, skyscrapers, airports, greenhouses, malls, and automobiles, and enhance the functionality of already utilized transparent surfaces. This is accomplished by exploiting the excitonic character of molecular and organic semiconductors that leads to "oscillator bunching" exhibiting uniquely distinct absorption spectra from the band-absorption of traditional inorganic semiconductors.

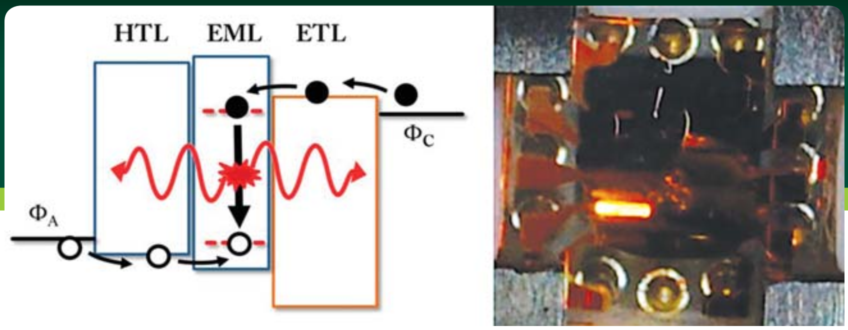

FIGURE 2. LEFT: Schematic energy-level diagram. RIGHT: Operation of a phosphorescent light-emitting diode.

Next-generation organic light emitting diodes for lighting. An important route to the reduction of green gasses lies in energy utilization. In particular, lighting accounts for about 17% of the total energy consumption in buildings. State of the art white organic light emitting diodes (WOLEDs) are currently poised to make reductions in this consumption rate for lighting as power efficiencies greater than that of fluorescent lighting have been demonstrated. However, WOLEDs are currently limited by external quantum efficiencies (EQE) of ~20% due to waveguided modes and are reliant on precious metal (Pt and Ir) containing phosphorescent dopants. To circumvent these shortcomings we are designing the next-generation devices based on phosphorescent nanostructured and abundant molecular materials.

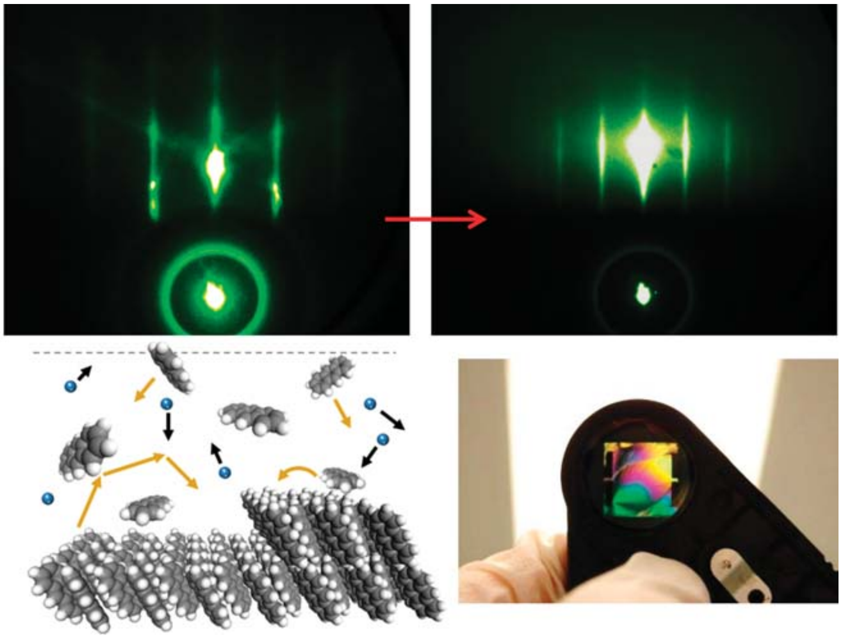

FIGURE 3. TOP: In situ grazing-incidence electron diffraction patterns of heteroepitaxial organic crystal growth. BOTTOM, LEFT: Schematic of molecular crystal growth dynamics. BOTTOM, RIGHT: Large area organic crystal films between two polarizers.

Understanding organic epitaxy. The presence of excitons in organic semiconductors at room temperature distinguish them from traditional semiconductors, providing exceptional opportunities for manipulating energy in a range of structures from light emitting diodes, lasers, transparent photovoltaics, and optical switches. However, control over crystalline order, orientation, and defect formation are crucial to the fabrication and optimization of these excitonic electronics. The overarching goal of understanding organic epitaxy is to explore bottom-up vapor-deposition routes to the growth of large-area organic and molecular crystalline films with enhanced properties.

RECENT PUBLICATIONS

C. Yang, R.R. Lunt, "Limits of visibly transparent luminescent solar concentrators," *Adv. Opt. Mat.* (invited, in print), 2016.

P. Chen, P. Kuttipillai, L. Wang, R.R. Lunt, "Homoepitaxial growth of metal halide crystals investigated by reflection high-energy electron diffraction," *Scientific Reports* (in print), 2016.

H. Yuan, R.R. Lunt, J.I. Thompson, R.Y. Ofoli, "Electrodeposition of Ni/Ni$(OH)_2$ catalytic films by cyclic voltammetry for the hydrogen evolution reaction," *Chem. Elect. Chem.* 3, 1–6, 2016.

D. Moghe, L. Wang, C.J. Traverse, A. Redoute, M. Sponseller, P.R. Brown, V. Bulović, R.R. Lunt, "All vapor-deposited lead-free $CsSnBr_3$ planar solar cells," *Nano Energy*, 28, 469–474, 2016.

Z. Tao, T.T. Han, F. Zhou, D. Torres, T. Wang, N. Sepulveda, K. Chang, M. Young, R.R. Lunt, C.-Y. Ruan, "The nature of photoinduced transition and metastable states in vanadium dioxide," *Scientific Reports*, 6, 38514, 2016.

L. Wang, D. Moghe, S. Hafezian, P. Chen, M. Young, M. Elinski, L. Martinu, S. Kéna-Cohen, R.R. Lunt, "Alkali metal halide salts as interface additives to fabricate hysteresis-free hybrid perovskite-based photovoltaic devices," *ACS Applied Materials & Interfaces*, 8, 35, 23086–23094, 2016.

M. Young, J.D. Suddard-Bangsund, T.J. Patrick, N. Pajares, S.Y. Lunt, and R.R. Lunt, "Organic heptamethine salts for photovoltaics and detectors with near-infrared photoresponse up to 1600 nm," *Adv. Opt. Mat.* 4, 7, 1028–1033, 2016.

P. Chen, R. Lunt, "Edge-nucleation driven hetero-quasiepitaxial growth of organic multilayer films," *Adv. Mat. Interfaces* 3, 17, 1600401, 2016.

A. Grossman, Y. Ding, R. Lunt, A. Bénard, "Solar photovoltaic design tool for non-residential buildings: from blueprints to arrays.," *Journal of Renewable and Sustainable Energy* 8, 035501, 2016.

H. Yuan, R.R. Lunt, G.J. Blanchard, and R.Y. Ofoli, "Synthesis of a MnO_x water oxidation catalyst on FTO by a novel dual-series cyclic voltammetry protocol," *Chem. Electro. Chem.* 3,5, 709–712, 2016.

Dennis Miller

Professor

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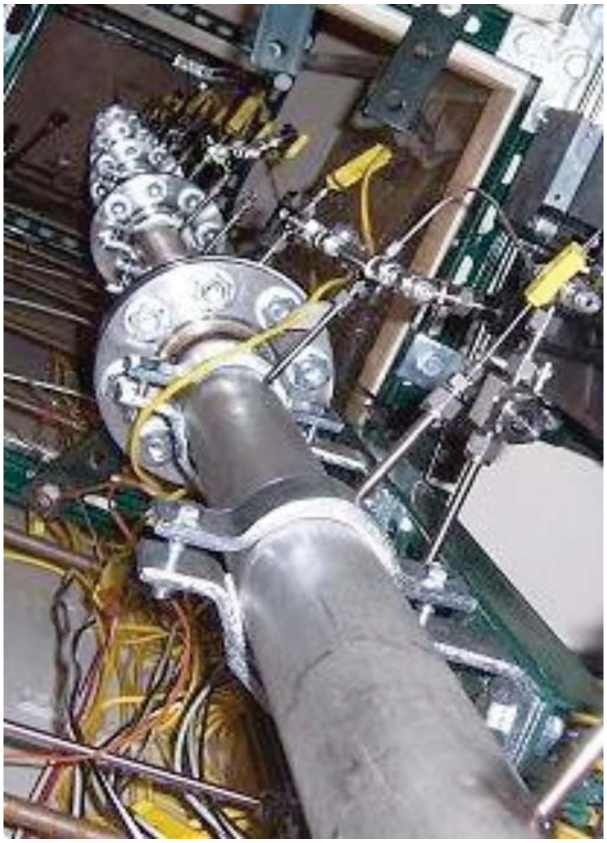


RESEARCH INTERESTS

Catalysis, chemicals from biomass, reactive separations

LABS

2535 Engineering Bldg., 2575 Engineering Bldg., MBI Pilot Plant

WEBSITES

http://www.chems.msu.edu/people/profile/millerd
http://www.chems.msu.edu/php/resproj.php?user=millerd

SPECIAL EQUIPMENT AVAILABLE

We have a pilot-scale reactive separations facility located at the MBI Building on campus. We have laboratory- and pilot-scale capabilities in catalysis, and a full slate of catalyst characterization instruments.

GROUP MEMBERS

RESEARCH STAFF: Lars Peereboom
GRADUATE STUDENTS: Aaron Oberg, Iman Nezam

RECENT PATENTS (23 TOTAL)

"An improved process for organic acid recovery from fermentation solutions," A. Orjuela, A. Yanez-McKay, C.T.Lira, D.J. Miller. US Patent 8,293,935 (10/23/2012).

"Process for producing mixed esters of fatty acids as biofuels," N. Asthana, D.J. Miller, C.T. Lira, E. Bittner. US Patent 8,613,780 (12/24/2013).

"Methods for making 1,3-dihydroxyacetone from glycerol," X. Hong, C.T. Lira, O. McGiveron, D.J. Miller. US Patent 8,735,633 (5/27/2014).

"Process for producing mixed esters of fatty acids as biofuels," N. Asthana, D.J. Miller, C.T. Lira, E. Bittner. US Patent 8,894,725 (11/25/2014).

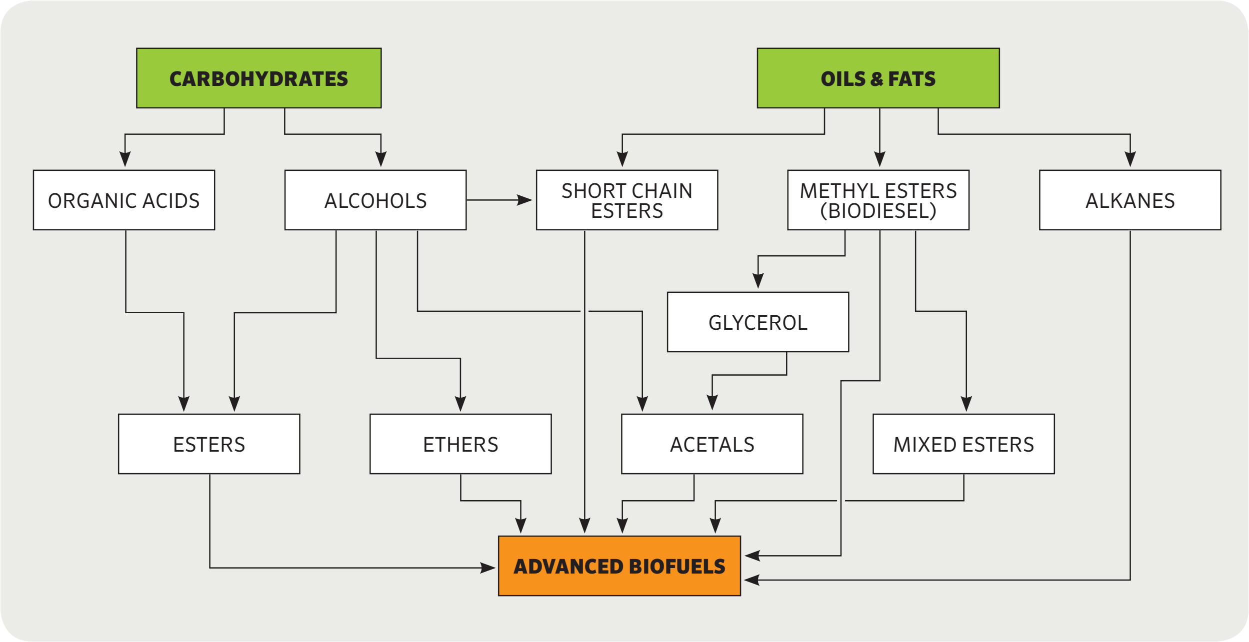
"Method for producing acyloxy carboxylic acids and derivatives thereof," D. Miller, C.T. Lira, L. Peereboom, A. Kolah. US Patent 9,090,556 (7/28/2015).

CURRENT RESEARCH

The supplementing of America's abundant fossil resources with fuels and chemicals derived from biomass remains important for generation of economic opportunities and for fostering national energy independence. In the laboratories of the Miller group, cutting-edge technology in heterogeneous catalysis and advanced processing is implemented to effectively convert biomass and biomass-derived intermediates to chemical products and fuels that compete with petroleum-based products in the current socio-economic environment.

The Miller group has examined a number of chemical systems directed at energy and materials production from renewable feedstocks. These have included the catalytic upgrading of biomass platform intermediates, mainly produced in fermentation processes, with the goal of building technical capabilities for the emerging biorefinery. In most cases, the overarching goal of the catalytic chemistry is deoxygenation of the biomass intermediate to a product that replaces a petroleum-derived counterpart. Classes of platform intermediates include carboxylic acids, sugar alcohols, linear alcohols, furanic compounds, and other derivatives; because these platform intermediates are typically of low volatility and are less thermally stable than their petroleum analogs, we have developed expertise in carrying out catalysis at mild temperatures under elevated hydrogen pressures in aqueous solution. The ability to design and prepare catalysts, characterize reaction pathways, and monitor chemical reaction kinetics have led to significant interactions with industrial partners, national laboratories, and agricultural groups.

The Miller group has partnered with the MSU engine group in mechanical engineering to produce and test advanced biofuels for internal combustion engines. Moving past today's first generation ethanol and biodiesel, emphasis has been placed on developing advanced biofuels with enhanced engine performance, high energy density, and storage and flow properties that facilitate their use as direct replacements for petroleum-derived fuels.



The Miller group uses reactive separations as a platform technology for process intensification. The group operates the MSU Reactive Distillation Facility, a full pilot-scale system consisting of two ten-meter reactive distillation columns located at MBI on the MSU campus. One column is glass for atmospheric pressure and vacuum operation; the second is stainless steel for elevated pressure studies. Reactive distillation is well-suited for reaction systems that are limited by chemical equilibrium, as the removal of one product by distillation allows the reaction to be driven to completion within the column. Current work emphasizes enhanced process intensification in reactive separation processes, including experimental and modeling studies of side reactors and energy integration.

RECENT PUBLICATIONS

A. Orjuela, C.T. Lira, D.J. Miller. “A novel process for recovery of fermentation-derived succinic acid: Conceptual design and preliminary economics,” *Bioresource Technology* 139, 235–241 (2013).

A. Santhanakrishnan, A. Shannon, L. Peereboom, C.T. Lira, D.J. Miller. “Kinetics of mixed alcohol esterification of butyric acid,” *Ind. & Eng. Chem. Res.*, 52, 1845–1853 (2013).

S. Kelkar, C.M. Saffron, Z. Li, S.-S. Kim, T.J. Pinnavaia, D.J. Miller, R. Kriegel. “Aromatics from biomass pyrolysis vapour using a bifunctional mesoporous catalyst.” *Green Chemistry* 16(2), 803 (2014).

Enquist-Newman, et al. (31 additional authors). “Efficient ethanol production from brown macroalgae sugars by a synthetic yeast platform,” *Nature* 505, 239–243 (2014).

F. Leyva, A. Orjuela, A. Kolah, C.T. Lira, D.J. Miller, G. Rodríguez. “Isoamyl propionate production by reactive distillation,” *Separation and Purification Technology* 146, 199–212 (2015).

T. Jordison, D.J. Miller. “Condensed phase ethanol conversion to higher alcohols,” *Ind. Eng. Chem. Res.*, 54, 10991–11000 (2015).

Donald Morelli

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RESEARCH INTERESTS
Materials physics, new semiconductors for energy applications, thermal and electronic transport in solids

LAB
Electronic Materials Laboratory (E172 Engineering Research Complex)

WEBSITE
www.egr.msu.edu/morelli-research

SPECIAL EQUIPMENT AVAILABLE
Equipment for synthesis of materials, including vacuum melting, arc-melting, and powder processing; x-ray diffractometer for crystal structure and phase identification; electrical and thermal transport property characterization from 80–1000K

GROUP MEMBERS
Jared Williams, Spencer Waldrop, Daniel Weller

CURRENT RESEARCH
Research in the Morelli group is aimed at designing, synthesizing, and characterizing new inorganic materials with applications in energy conversion. Currently, two main thrusts or our research are (1) investigation of new thermoelectric materials for conversion of heat to electricity; and (2) development of new materials for cryogenic cooling of Peltier devices for space-based applications.

The Center for Revolutionary Materials for Solid State Energy Conversion, a US Department of Energy–funded research center led by MSU, focuses on solid state conversion of thermal energy to useful electrical power, both to increase the efficiency of traditional industrial energy processes and to tap new unused sources of energy such as solar thermal. Additionally materials with enhanced thermoelectric properties will find application in high efficiency, environmentally benign climate control systems. We are undertaking a broad-based effort in semiconductor energy conversion materials utilizing and combining experimental, theoretical, and computational efforts. A major focus of our effort will be in the synthesis of new forms of matter, including both single phase alloys and compounds and composite structures created using nanoscience.

Ultimately, by working together in this Center we aim to develop design rules to predict properties of advanced thermoelectric materials, and realize these structures through innovative synthesis and advanced structural as well as chemical characterization.

Some examples of current work in our group include:

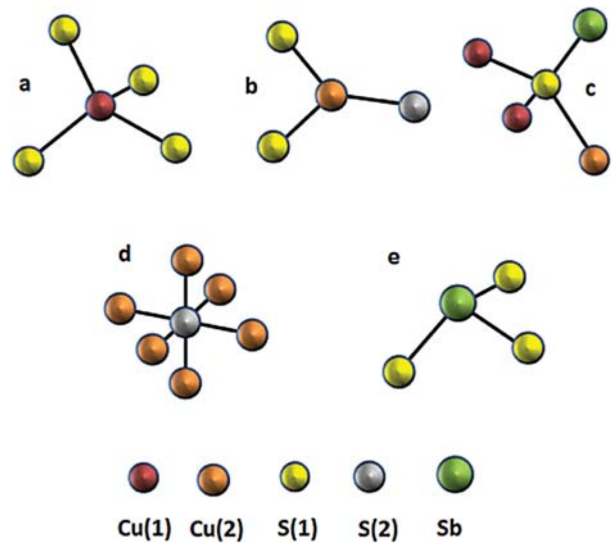

FIGURE 1. Structural sub-units in the thermoelectric compound tetrahedrite. The structure is characterized by (A) tetrahedrally coordinated Cu (1); (B) trigonally coordinated Cu(2); (C) tetrahedrally coordinated S(1); (D) octahedrally coordinated S(2); (E) trigonally coordinated Sb. Electronic and thermal transport properties are determined by the detailed nature of structure and bonding in this material.

Understanding the relationship between structure and bonding and the thermal conductivity of solids. Good thermoelectric materials have very low thermal conductivity, and if we can understand how to control this parameter, new materials can be designed with improved properties. In collaboration with colleagues in our Center, we have combined state-of-the-art computational approaches with thermal and electronic transport characterization to study the relationship between crystal structure and proeprties of a class of promising semiconductors (Figure 1). We find that certain types of structural arrangements of atoms give rise to strongly anharmonic lattice vibrations, a key ingredient in determining a material's heat conduction characteristics. We have synthesized these predicted structures in the laboratory and verified the predictions of these computational models.

Thermoelectric materials synthesized from earth-abundant sources. We have shown that the mineral tetrahedrite (Figure 2) can be used directly as a thermoelectric material with very little compositional modification. Tetrahedrite, of chemical formula $Cu_{12}Sb_4S_{13}$, is the most common sulfosalt mineral on Earth, and its use as a source thermoelectric material could pave the way to large scale and low cost application of thermoelectricity for energy conversion. We have found that the mineral itself can be used directly in a powder processing methodology to synthesize materials with large

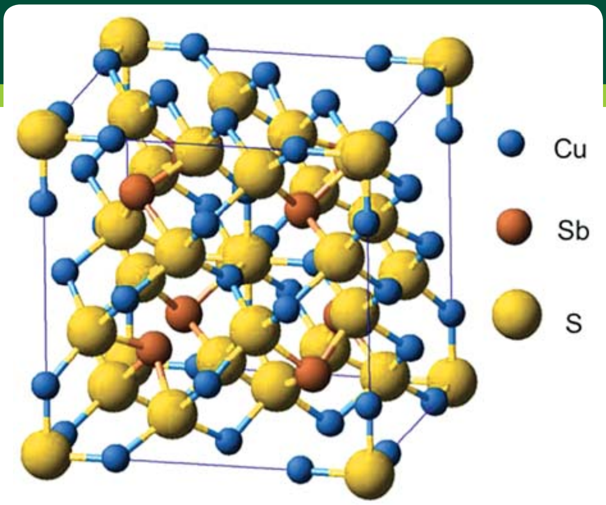

FIGURE 2. A natural mineral tetrahedrite polycrystal (*left*). This compound is the most widespread sulfosalt on earth; it is also a semiconductor whose properties can be tailored to produce high thermoelectric figure of merit. The crystal structure of this compound is shown on the right.

thermoelectric figure of merit in a temperature range suitable for the conversion of waste heat from a variety of sources, including vehicle exhaust gas and power plant discharge sources.

Thermoelectrics for cooling of infrared sensors. Our group has also been investigating new materials for low temperature Peltier devices. These devices can be used to cool infrared sensors on satellites to the cryogenic temperatures necessary for them to operate. We are exploring thermoelectric effects below room temperature in alloys comprised of elements containing f-shell electrons. Two new compounds of particular interest are $YbAl_2$ and $YbCu_2Si_2$. We have found that by chemical substitution the magnitude of the Seebeck coefficient can be increased, and the temperature at which it is maximized can be controlled. This provides a means of improving and optimizing the thermoelectric properties in the cryogenic temperature range.

RECENT PUBLICATIONS

M. Beekman, D.T. Morelli, G.S. Nolas. "Better thermoelectrics through glasslike crystals," *Nature Materials* 14, 1182 (2015).

D. James, X. Lu, D.T. Morelli, S.L Brock, "Solvothermal synthesis of tetrahedrite: speeding up the process of thermoelectric material generation," *Applied Materials and Interfaces* 7, 23623 (2015).

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W. Lai, Y. Wang, D.T. Morelli, and X. Lu. "From bonding asymmetry to angharmonic rattling in $Cu_{12}Sb_4S_{13}$ tetrahedrites: when lone-pair electrons are not so lonely," *Advanced Functional Materials* 25, 3648 (2015).

G.J. Lehr, D.T. Morelli, H. Jin, J.P. Heremans. "$YbCu_2Si_2$-$LaCu_2Si_2$ solid solutions with enhanced thermoelectric power factors," *Journal of Electronic Materials* 44, 1663 (2015).

V. Ponnamblam, D.T. Morelli. "Thermoelectric investigation of the pseudo-binary system $PbTeCoSe_2$," *Journal of Electronic Materials* 44, 2089 (2015).

W. Carr, D.T. Morelli. "Influence of doping and solid solution formation on the thermoelectric properties of chalcopyrite semiconductors," *Journal of Alloys and Compounds* 630, 277 (2015).

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X. Lu, D.T. Morelli, Y. Xia, V. Ozolins. "Increasing the figure of merit of tetrahedrites by co-doping with nickel and zinc," *Chemistry of Materials* 27, 408 (2015).

S. Waldrop, D.T. Morelli. "Low temperature thermoelectric properties of $PbSb_{2-x}Te_x$ for cryogenic Peltier cooling applications," *Journal of Electronic Materials* 44, 1562 (2015).

X. Lu, D.T. Morelli. "The effect of Te substitution for Sb on thermoelectric properties of tetrahedrite," *Journal of Electronic Materials* 43, 1983 (2014).

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Y. Zhang, V. Ozolins, D.T. Morelli, C. Wolverton, "Prediction of new stable compounds and promising thermoelectrics in the Cu-Sb-Se system," *Chemistry of Materials* 26, 3427 (2014).

Ramani Narayan

University Distinguished Professor

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RESEARCH INTERESTS

Design and engineer biobased and biodegradable-compostable plastics, develop environmentally responsible end-of-life options for plastics and bioplastics materials, conduct carbon footprint and life cycle assessment (LCA) of materials, studies in reactive extrusion processing and biofiber composites

LAB

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GROUP MEMBERS

POSTDOCTORAL & VISITING RESEARCH FELLOWS: Dr. Mohan Patil (UICT, India), Dr. Elodie Hablot (Univ. of Strasbourg, France), Dr. Yuya Tachibana (AIST, Japan), Professor Philippe Dubois (Univ. of Mons, Belgium), Professor Y.Z. Wang (Sichuan Univ., China), Dr. Jean Marie (Ben) Raquez (Univ. of Mons, Belgium), Dr. Weipeng Liu (Green Star company, China). STUDENTS: graduated 19 Ph.D and 20 Master's students; currently 5 graduate students and 8 undergraduates work in the group.

CURRENT RESEARCH

Biobased Materials (Narayan) Research Group design and engineer new biobased and biodegradable-compostable polymer materials and bio processes using agricultural crops and residues (soybean and corn), lignocellulosic biomass, and algae. These biobased products find commercial application in films for plastic bags, injection molded articles, thermoformed products, foamed sheets for protective and insulation packaging, and The group's biobased materials technology platform is covered by 29 patents; 200 peer reviewed publications, and several technologies have been licensed or resulted in a spin-off company. Successful technology commercialization exemplars are:

- poly(lactic acid) (PLA) technology—the world's foremost 100% biobased and biodegradable-compostable material—with a 150,000-ton commercial plant operating in Blair, Nebraska, by NatureWorks LLC (www.natureworksllc.com)
- biopolyester and modified PLA resins for biodegradable-compostable films, molded products, and engineering plastics through Northern Technologies (www.natur-tec.com), a $150 million NASDAQ traded company
- biofoam sheet manufacturing for cushion and insulation packaging under the trade name GreenCell by KTM Industries (www.ktmindustries.com)
- biobased polyols technology for flexible and rigid polyurethanes in partnership with a Michigan agribusiness, Zeeland biobased products (www.zfsinc.com)
- licensing four patents on thermoplastic modified starch and its copolymers with biopolyesters to Ingredion Inc., a $2.3 billion international company.

FIGURE 1.

The major R&D and technology commercialization effort underway is building an industrial soybean based biorefinery producing value added industrial products in Michigan in cooperation with Zeeland Farm Services (www.zfsinc.com). ZFS is Michigan's largest soybean processor servicing about 2500 Michigan farmers and processing 26,000 bushels of soybean (1.56 million pounds) per day—representing 99% of the soybeans grown in the State. Currently they produce two products namely soybean meal used as animal feed, and oil which is used in food applications. Diversifying the product base with higher value industrial products provides more economic stability and job creation to the Michigan economy. We developed an ozonolysis technology platform to convert the fatty acid methyl esters derived from soybean oil to C-9 diesters and C-9, C-7 monoesters which have industrial applications. The plant oils are being converted into biobased polyols which is used in making flexible polyurethanes for automotive and industrial applications.

The soymeal residue remaining after removing the oil by solvent extraction is rich in proteins and carbohydrates. We are developing technology to make rigid polyurethane foams. Figure 2 shows samples: A is reference formulation with no soy polyol; B contains 25% and C contains 50% of soy polyol. Another synthetic strategy being developed is to convert the

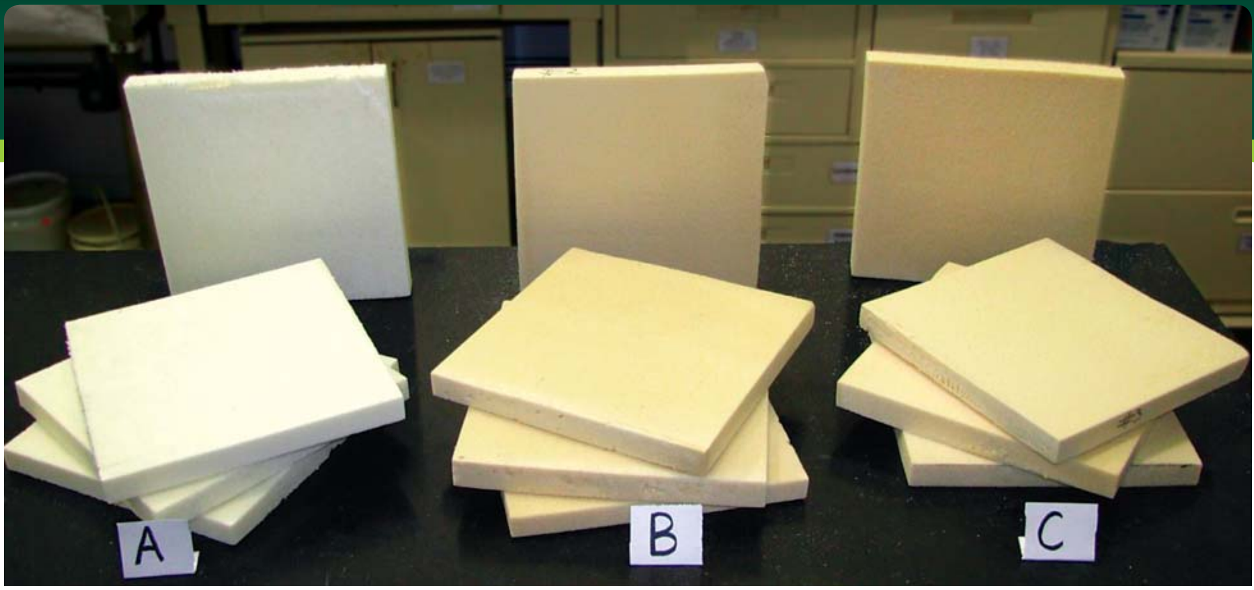

FIGURE 2. Samples of rigid polyurethane foams: (A) reference formulation with no soy polyol, (B) contains 25% soy polyol, (C) contains 50% soy polyol.

soy meal to polyurethane building blocks by eliminating or reducing the use of the toxic isocyanate reagent.

Our biobased and biodegradable-compostable hybrid materials technology platform is based on poly(lactide) (PLA) resins derived from plant-biomass feedstock like corn and sugarcane. Funded by NSF SBIR Phase I and II grants, the technology is being commercialized by Natur-Tec, a business unit of Northern Technologies (NASDAQ:NTIC). The company currently supplies biodegradable-compostable bags to global companies such as Levi Strauss & Co. About 76,000 m.t./yr of plastic packaging resins are used for packaging 5 billion garments in South Asia alone (Figure 3), translating to about $200 million in economic value.

The group is working towards addressing the major issue of microplastics in the ocean environment. In a recent paper published in the journal *Science* (February 2015, Vol. 347, No. 6223, pg. 768), we reported that 4.8 to 12.7 million tons of plastics entered into the oceans in 2010 and without any intervention would increase to 10.4 to 27.7 million tons by 2025. The paper shows that reducing 85% of waste from the top 35 mismanaged waste countries would result in a 75% reduction of plastic waste going into the oceans. We are working towards developing and implementing compostable plastics technology in conjunction with composting and anaerobic digestion systems to prevent "mismanaged plastic waste" from entering into the oceans (Figure 4). These efforts along with along with educational and consumer awareness messaging can clearly advance the goal to "a cleaner ocean environment."

FIGURE 3.

FIGURE 4.

RECENT PUBLICATIONS

S. Dewasthale, D. Graiver, R. Narayan. "Biobased interpenetrating polymers networks derived from oligomerized soybean oil and polydimethylsiloxane," *Journal of Applied Polymer Science*. 132(13) (2015).

A. Grabowski, S.E.M. Selke, R. Auras, M.K. Patel, R. Narayan. "Life cycle inventory data quality issues for bioplastics feedstocks," *International Journal of Life Cycle Assessment* (2015).

Y. Tachibana, X. Shi, D. Graiver, R Narayan. "The use of glycerol carbonate in the preparation of highly branched siloxy polymers," *Silicon*. 7(1):5–13 (2014).

E. Hablot, S. Dharmalingam, D.G. Hayes, L.C. Wadsworth, C. Blazy, R. Narayan. "Effect of simulated weathering on physicochemical properties and inherent biodegradation of PLA/PHA nonwoven mulches," *Journal of Polymers and the Environment*. 22(4):417–429 (2014).

R.Narayan. "The facts about biodegradable plastics," *Resource Recycling*. 33(1):32–36 (2014).

R. Narayan. "Principles, drivers, and analysis of biodegradable and biobased plastics," in *Handbook of Biodegradable Polymers,* 2nd edition, ed. C. Bastioli, Smithers Rapra Technology (November 2014).

Jason Nicholas

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RESEARCH INTERESTS

Solid oxide fuel cells, mechano-chemical coupling, oxidation resistance alloys, chemical separators, chemical reactors, cost-effective processing methodologies, chemical sensors, batteries, chemical actuators, pseudo-capacitors, electro-chromic coatings, nano-composite electrode modeling, micro-structural optimization.

LAB

Solid State Ionics Laboratory, 172 Energy and Automotive Research Laboratory

WEBSITE

https://www.egr.msu.edu/nicholasgroup/index.php

SPECIAL EQUIPMENT AVAILABLE

1200°C controlled atmosphere *in situ* curvature measurement system, 1600°C controlled atmosphere dilatometer (Netzsch 402C), 1600°C controlled atmosphere TGA-DSC (Netzsch Jupiter 449 F5)

GROUP MEMBERS

COLLABORATORS: Yue Qi, Thomas Bieler, Richard Lunt.

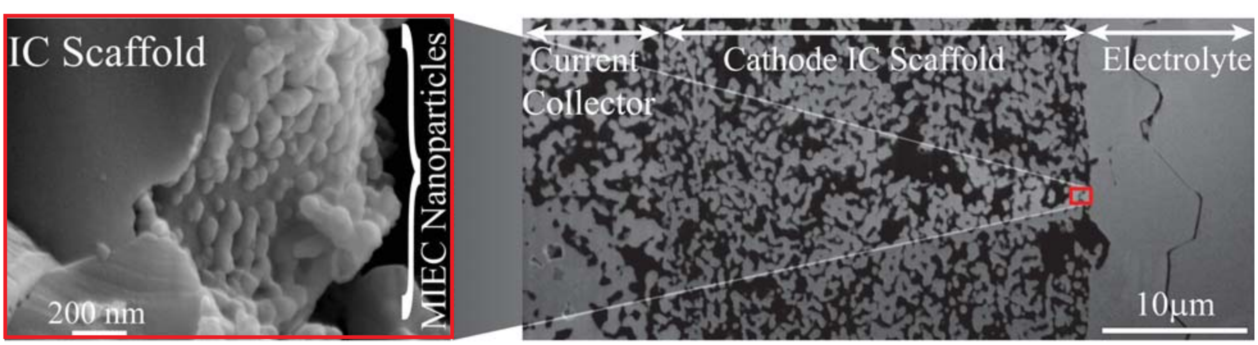
STUDENTS: Eric Straley, Yuxi Ma, Yubo Zhang, Quan Zhou, Brandon Bocklund

CURRENT RESEARCH

Solid oxide fuel cell research. Solid Oxide Fuel Cells (SOFCs) are a promising green energy technology offering high chemical to electricity conversion efficiencies, the ability to both store and produce energy, and a possible path to transition from today's hydrocarbon-based economy to a CO2-neutral economy running on hydrogen, solar fuels, or biofuels. Unfortunately, traditional SOFCs have been restricted to operating temperatures in excess of 750°C. To better understand intrinsic SOFC material behavior and reduce SOFC operating temperatures, our group has focused on (A) mechano-chemical coupling in electro-chemically active solids, (B) computationally-led SOFC braze development and (C) nano-composite Solid Oxide Fuel Cell (SOFC) electrode enhancement. Some of our recent accomplishments include the publication of most highly cited gadolinium doped ceria sintering aid paper of the last decade, the development of the world's most highly cited nano-composite Solid Oxide Fuel Cell electrode model (the SIMPLE model), and the development of a new in situ, electrode-free bilayer curvature relaxation technique for measuring oxygen surface exchange coefficients as a function of simultaneously measured stress state. Updates on our research can be found at https://www.egr.msu.edu/nicholasgroup/simple.php.

Mechano-chemical coupling. Materials capable of quickly exchanging oxygen with the surrounding atmosphere are used in a variety of electrochemical devices such as solid oxide fuel cells (SOFCs), catalytic converters, gas sensors, solar thermochemical fuel generators, and gas separation membranes. In these applications, overall device performance is often limited by the rate of oxygen exchange with the atmosphere; a process quantified by the oxygen incorporation reaction chemical rate coefficient, *k*. Unfortunately, large disparities exist in the reported k's of even the most common oxygen exchange materials. For instance, literature reports indicate that there is a 2-orders-of-magnitude variation, a 3-order-of-magnitude variation, and a 4-order-of-magnitude variation in the 650°C *k* of CeO_{2-x}, lanthanum strontium cobalt iron oxide ($La_{0.6}Sr_{0.4}Fe_{0.8}Co_{0.2}O_{3-\delta}$), and $La_{0.6}Sr_{0.4}FeO_{3-\delta}$ (LSF64), respectively. Many authors have suggested that some of this *k* variation may be caused by varying MIEC stress/strain states and/or electrode effects. However, electrode-free techniques capable of simultaneously measuring a material's *k* and stress state have been missing from the literature. To remedy this problem, our group has developed a new curvature relaxation technique to measure the oxygen surface exchange coefficients and stress states of dense, porous, thin, or thick film oxygen exchange materials. This new, *in situ/in operando* technique is presently among the cheapest electrode-free techniques for measuring oxygen surface exchange coefficients, and is the only technique yielding simultaneous *k* and stress data.

FIGURE 1. Scanning electron micrograph of a SOFC cathode made of mixed ionic electronic conducting (MIEC) infiltrate atop an ionic conducting (IC) scaffold.



Durable, impermeable SOFC brazes. Traditional Ag/CuO SOFC brazes exhibit detrimental pore formation caused by wetting problems during manufacturing, the reduction of CuO during operation in hydrogen, and water vapor formation within the braze. The objective of this work is to design and test new, SOFC-compatible, silver-free brazes forming durable, oxygen and/or hydrogen impermeable protective surface scales. Computational efforts to identify promising new braze compositions are being led by the research group of Dr. Yue Qi, while the Nicholas Group and the group of Dr. Thomas Bieler are leading experimental studies aimed at characterizing new braze and braze oxide compositions.

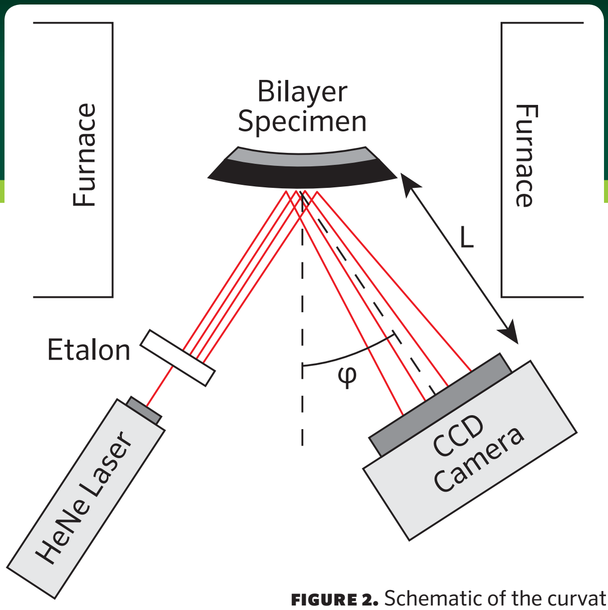


FIGURE 2. Schematic of the curvature relaxation apparatus.

Infiltrated nano-composite SOFC electrode optimization. Nano-composite SOFC cathodes produced by the infiltration and subsequent firing of nitrate solutions have exhibited some of the best low-temperature performance ever reported. Unfortunately, it has been difficult to control the size of nanoparticles obtained via the infiltration method. For instance, a survey of the recent literature indicates that 22 studies had infiltrated particle sizes ranging from large 100–200 nm, 17 studies had infiltrated particle sizes ranging from 50–80 nm, five studies had infiltrated particle sizes ranging from 30–40 nm, and five studies had nano-particle sizes less than 30 nm in diameter. This inability to control infiltrated nano-particle has restricted most nano-composite SOFC cathodes to operating temperatures >>600°C. Research our group has shown that infiltrate particle sizes can either be controllably modulated from 21 to 48 nm through the pre-infiltration of nano-ceria, or from 17 to 48 nm by desiccating precursor nitrate gels in atmospheres containing varying amounts of water. The cathodes produced with these techniques reached a 0.1 Ωcm^2 commercialization target at 540°C, making them some of the best performing (if not the best performing) infiltrated SOFC cathodes ever produced.

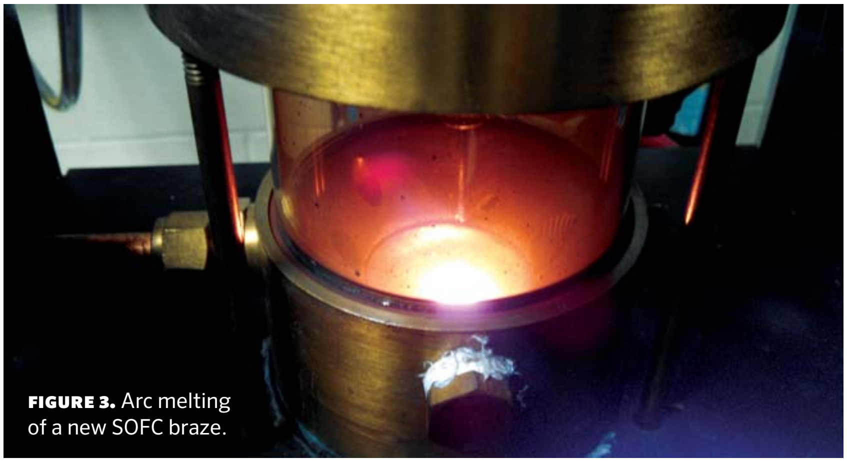


FIGURE 3. Arc melting of a new SOFC braze.

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T.E. Burye, J.D. Nicholas. "Nano-ceria pre-infiltration improves $La_{0.6}Sr_{0.4}Co_{0.8}Fe_{0.2}O_{3-x}$ infiltrated solid oxide fuel cell cathode performance," *Journal of Power Sources* 300: 402–412 (http://dx.doi.org/10.1016/j.jpowsour.2015.09.080) (2015).

T.E. Burye, J.D. Nicholas. "Improving $La_{0.6}Sr_{0.4}Co_{0.8}Fe_{0.2}O_{3-\delta}$ infiltrated solid oxide fuel cell cathode performance through precursor solution desiccation," *Journal of Power Sources* 276: 54–61 (http://dx.doi.org/10.1016/j.jpowsour.2014.11.082) (2015).

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Robert Y. Ofoli

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RESEARCH INTERESTS

Sustainable production of fuels and chemicals from renewables: biomass to chemicals and high density liquid fuels; biomimetic water oxidation to produce hydrogen and organic molecules

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SPECIAL EQUIPMENT AVAILABLE

CHI 660D electrochemical workstation

GROUP MEMBERS

STUDENTS: Matthew Hames. COLLABORATING FACULTY: Gary Blanchard (Chemistry), James Jackson (Chemistry), Richard Lunt, Dennis Miller, Yirong Mo (Chemistry, Western Michigan), Sherine Obare (Chemistry, Western Michigan)

CURRENT RESEARCH

Our research focuses on the use of nanostructured biomimetic catalysts for sustainable production of chemicals and high-density liquid fuels. We integrate rational catalyst design and synthesis, characterization and assessment, and modeling and simulation to understand structure-functional relationships. We work on two thrusts of significant scientific and societal interest: biomimetic water oxidation to produce hydrogen and organic materials; and transformation of biorenewables to chemicals and high-density liquid fuels. Our eventual goal is to produce materials that are equivalent to those from petroleum-based raw materials.

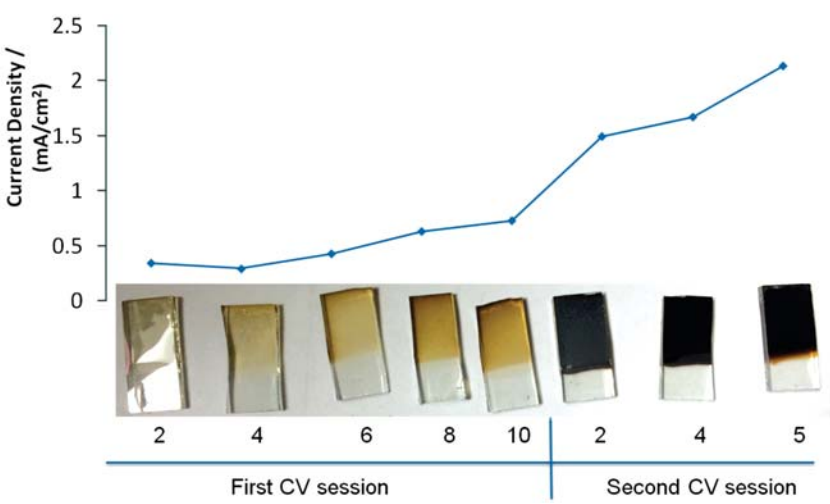


FIGURE 1. Functionality assessment after selected stages of electrodeposition. The gradual increase in peak current density during the first CV series increases dramatically during the second CV series, likely the result of continued enhancement in the oxidation state of the catalyst. The slope of the functionality curve during the second session is strongly positive, giving indication of further enhancement in oxidation state.

Biomimetic water oxidation to produce hydrogen fuel. The sun provides a clean and sustainable source of energy. However, its intermittency requires development of storage strategies to enable its use on demand. Solar-driven electrocatalytic water splitting, which converts solar energy into chemical energy for storage as fuel hydrogen, can effectively mitigate the intermittence of solar radiation. Water splitting consists of two half reactions: water oxidation and hydrogen evolution. Both reactions rely on highly effective electrocatalysts. Our work has focused on developing highly effective low-cost electrocatalysts for both reactions.

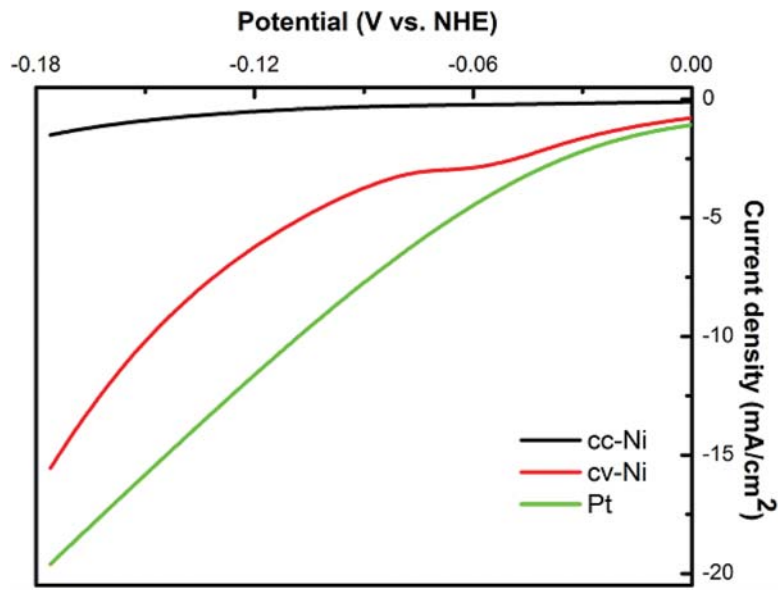
We have developed an electrochemical method to immobilize a cobalt-based (Co-OXO) water oxidation catalyst on a conductive surface to promote recyclability and reusability without affecting functionality. We have also developed a method to synthesize manganese-based (MnO_x) catalytic films in situ, generating a nanoscale fibrous morphology that provides steady and excellent water oxidation performance. The new method involves two series of cyclic voltammetry (CV) over different potential ranges, followed by calcination to increase crystallinity. This work has the potential to open routes for synthesizing and optimizing other manganese-based water oxidation catalysts (Fig. 1).

We have investigated the feasibility of incorporating manganese-based water oxidation catalysts into TiO_2 to build a composite photoanode. Results show that the composite photoanode has good activity under ultraviolet (UV) illumination, and that its catalytic performance can be significantly improved by enabling solar energy collection over a wider range of wavelengths.

We have also developed a new electrodeposition method to synthesize $Ni/Ni(OH)_2$ catalysts in situ on conductive surfaces For the hydrogen evolution reaction. The new method involves two cycles of CV over a single potential range. This new inexpensive method involves a single CV scan of two potential ramps ranging from 0 to –1.2 V, and produces a catalytic film with a uniform surface morphology consisting of an evenly-distributed monolayer of spherical walnut-shaped particles. The film is stable, has a much better catalytic performance than traditional cc-Ni HER catalyst or Ni foil. A particularly important contribution of this work is that the new method creates a large number of $Ni(OH)_2/Ni$ interfaces, leading to a catalytic performance that shifts significantly towards that of platinum (Fig 2).

Catalytic transformation of biorenewables to high-density liquid fuels. Global energy will increase significantly over the next few decades. Even with new sources made possible by

FIGURE 2. Functionality test showing that the performance of the new catalyst (cv-Ni) shifts significantly towards that of platinum.



such technologies as fracking, it is generally believed that future petroleum supplies will not completely meet global needs. This has created a critical need for the sustainable production of fuels and chemicals. Solar energy is an important source for meeting global demand, because of the quantity incident on the planet. However, even if technological challenges are addressed to make solar energy a mainstream source, it will be difficult to meet the demand for high energy density liquid fuels. This will, instead, fall on biomass conversion and subsequent exhaustive reduction.

The goal of our research is to help address this critical need. We report here on an effective protocol for synthesizing monodisperse ruthenium nanoparticles (Ru NPs) supported on mesoporous silica (MSU-F), using octadecylamine (ODA) as stabilizer, for the aqueous phase hydrogenation of the α-keto site of pyruvic acid (PyA). The facile phase-transfer protocol is a reliable method to obtain stable sub-10nm Ru colloidal NPs. The ODA-stabilized Ru NPs are well-dispersed following in situ deposition on ordered mesoporous silica (MSU-F). We used three different thermal procedures to activate the supported Ru nanocatalysts, each maintaining the uniform distribution of nanoparticles on the supports. Gentle thermal oxidation enables complete ODA decomposition, but does not remove the decomposed residuals. Thermal reduction allows complete decomposition and removal of ODA, but results in some loss of Ru nanoparticles. Argon-protected calcination is the most efficient activation method, because it removes the ODA completely while modifying the surface structure of the support, and facilitating the metal-support interaction.

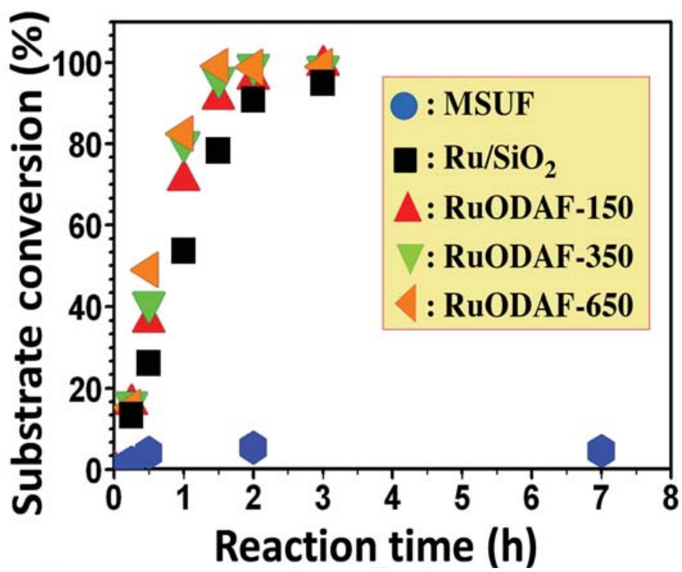


FIGURE 3. PyA hydrogenation over pure support, commercial catalyst, and ODA-stabilized Ru catalysts. Reaction conditions: T = 45°C; P(H_2) = 5.0 bar.

RECENT PUBLICATIONS

H. Yuan, R.R. Lunt, J.I. Thompson, R.Y. Ofoli, "Electrodeposition of Ni/Ni$(OH)_2$ catalytic films for the hydrogen evolution reaction produced by using cyclic voltammetry," *ChemElectroChem* (doi: 10.1002/celc.201600572) 2016.

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X. Ma, R. Lin, C. Beuerle, J.E. Jackson, S.O. Obare, R.Y. Ofoli, "Effects of surface activation on the structural and catalytic properties of ruthenium nanoparticles supported on mesoporous silica," *Nanotechnology* 25(4), Article 045701 (2014).

Charles Petty

Professor

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RESEARCH INTERESTS

Transport phenomena (single phase and multiphase); rheology of suspensions, turbulent flows in rotating and nonrotating frames, hydrocyclone classifiers and separators, animal orientation and navigation, computational transport phenomena for undergraduates

CURRENT COLLABORATING STUDENTS

Andrew Bowden (Chemical Engineering, Undergraduate Professorial Assistant), Devinda Wijewardena (Chemical Engineering, Undergraduate Professorial Assistant), Abdul Motin (PhD Candidate, Mechanical Engineering, A. Bénard, Advisor)

CURRENT COLLABORATING FACULTY AND COLLEAGUES

Dr. YoChan Kim (PhD 2006, MSU, Bechtel National), Dr. Karuna Koppula (PhD 2009, MSU, Rochester Institute of Technology), Dr. André Bénard (Mechanical Engineering, MSU), Dr. Vlad Tarabara (Environmental Engineering, MSU), Dr. Farhad Jaberi (Mechanical Engineering, MSU)

NSF INDUSTRY/UNIVERSITY COOPERATIVE RESEARCH CENTER, 2004–2011

C. Petty and A. Bénard, Founders and Co-Directors, Michigan State University, University of Tulsa, Central Florida University, University of Akron, Ansys, Bechtel, BP, CD-adapco, Chevron, ConocoPhillips, M-I Swaco, Petrobras, Pfizer, National Science Foundation, Department of Interior (MMS).

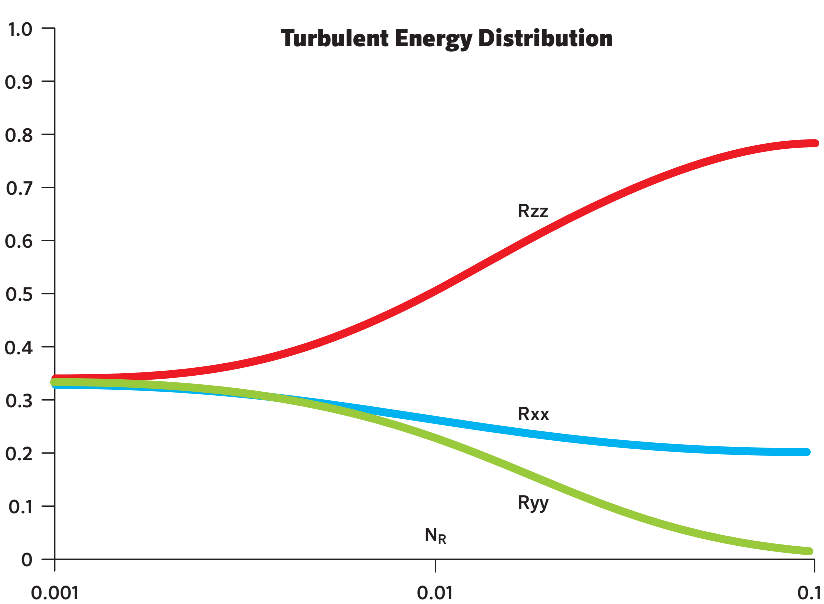


FIGURE 1. Redistribution of turbulent kinetic energy among the three components of the velocity in rotating shear flows (K. Koppula, PhD, Chemical Engineering, 2009, MSU).

PATENT

"Improved Hydrocyclone," C.A. Petty, R.G. Dvorak, H.C. Chen. US Patent 4,855,066, Michigan State University (1989).

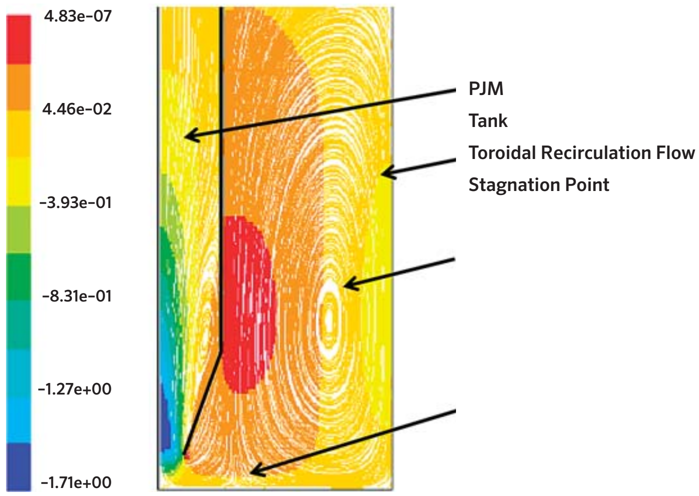
CURRENT RESEARCH

Multiphase transport phenomena research and education. Multiphase fluids (i.e., drilling fluids, foodstuffs, pharmaceuticals, blood, liquid crystalline polymers, aerosols, fuel sprays, oil/water dispersions, solid/liquid suspensions, liquid/gas mists, and bubbly liquids) occur ubiquitously in many applications in engineering, polymer science, human medicine, and biology. Computational methods can provide significant insights related to the behavior of these fluids in extreme conditions and in complex geometries. Examples include hydrate formation in subsea pipelines; oil/water spills in the ocean; dust storms on Earth and on Mars; circulation of large scale ocean currents; mixing of pollutants in lakes and rivers; ice formation in the atmosphere; particle deposition in the lungs; and, effluent flows from hydrocyclone separators.

Flows of multiphase fluids are often unstable and involve large-scale secondary motions that can significantly influence multiphase mixing and separation, interfacial mass and heat transfer, and multiphase reactions. Professor Petty and his colleagues are interested in the further development and experimental validation of next generation multiphase transport phenomena closure models and the further development of computational transport phenomena methods for rapid analysis and design of processes with an emphasis on safety.

Turbulent fluctuations and bird navigation . The solution of the Reynolds-Averaged Navier-Stokes equation is the only viable means for simulating high Reynolds number flows typically encountered in engineering practice and in the troposphere. Research at MSU for the past twenty years has developed a realizable, algebraic Reynolds stress closure for rotating and nonrotating turbulent flows. The theory predicts the redistribution of turbulent kinetic energy among the three components of the velocity in simple mean shear flows (see Figure 1). The new approach is being used to analyze atmospheric scintillation of electromagnetic waves induced by the local coupling between the angular velocity of Earth and fluctuations in the turbulent velocity field. The relationship between scintillation phenomena and bird migration may provide an explanation of a longstanding question in biology: How do birds navigate over global scales?

Cross flow filtration hydrocyclone for liquid/liquid separation. A cross flow filtration hydrocyclone (CFFH) combines the desirable attributes of a vortex separator and a filter. By selecting a hydrophilic filter medium, a CFFH clarifier has the potential to produce a filtrate phase with a low concentration of a dispersed organic phase in a single stage. The CFFH concept may provide a practical means to mitigate three problems associated with current hydrocyclone clarifiers: 1) the loss of separation performance due to core flow reversal; 2) the loss of separation performance due to entrained particles in the sidewall boundary layer; and, 3) the loss of separation performance due to turndown. The third feature may be the most significant inasmuch as the CFFH environment provides a self-regulating means to reduce the local filtrate flux across the sidewall filter. The CFFH concept for produced water can be extended to crude oil dehydration, to liquid/liquid separation of concentrated phases encountered in liquid/liquid extraction applications, and to downhole and subsea separation of oil and water. The objective of current research is to develop a prototype oil/water separator for field testing.



Multiphase flows. Particle-laden flows are widely encountered in the oil and gas industry. An accurate description of particle transport in turbulent flows is of great importance for predicting fouling of various equipment as well as erosion of pipe walls. As illustrated by the jet-pulsed mixer shown below (Figure 2) and flow through a bend (Figure 3), deposition of particles on the walls is influenced significantly by streamlines curvature of the flow field.

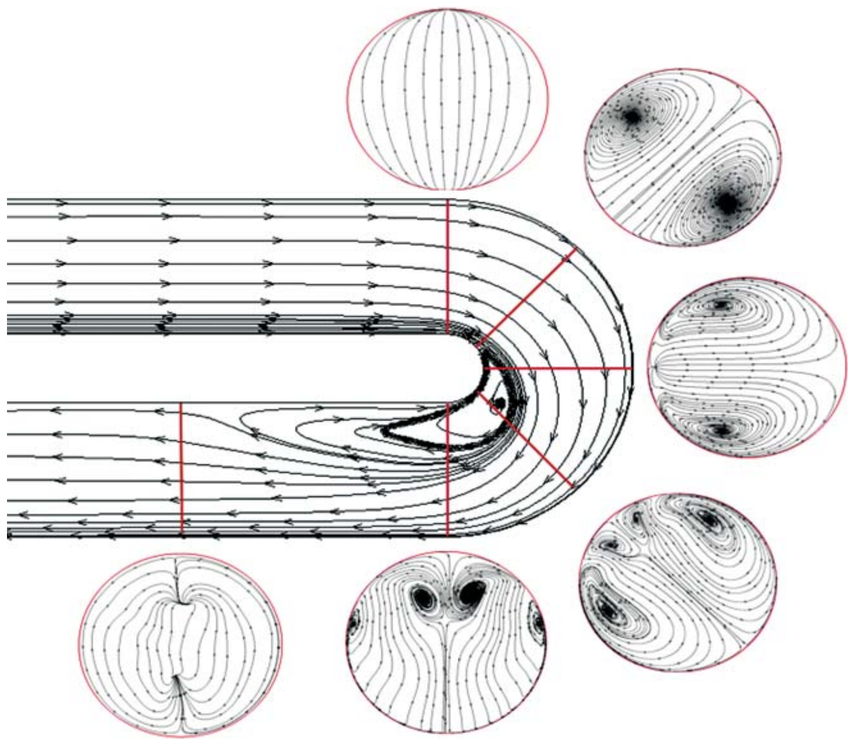


FIGURE 2 (*right, top*). Path lines colored by axial velocity (m/s) at 5 seconds into Cycle 4 (suction phase). Note the toroidal secondary flows within the PJM as well as in the tank. (NSF/Combined Research and Curriculum Development Case Study. D. Eldein, S. Teich-McGoldrick, J. Roth, and C. Trainer. “CFD Simulation of a Pulsed-Jet Mixer,” Second Place Ribbon: Undergraduate Poster Session, Annual AIChE Meeting, 3–8 November 2002, Indianapolis, Indiana)

FIGURE 3 (*right, bottom*). Flow patterns through a bend (180o) with cutouts that show various recirculation patterns at different cross-sections. The turbulence model and the wall functions strongly influence the qualitative accuracy of the simulation (P. Zhang, PhD, Mechanical Engineering, 2012, MSU).

RECENT PUBLICATIONS

Y. Kim, A. Bénard, C.A. Petty. “Microstructure and rheology of rigid rod suspensions,” *Ind. Eng. Chem. Res.*, Special Issue, Scott Fogler Festschrift, 2015. (doi: 10.1021/ie503995y)

K.S. Koppula, S. Muthu, A. Bénard, C.A. Petty. “The URAPS closure for the normalized Reynolds,” *Physica Scripta*, T155 (2013).

K.S. Koppula, A. Bénard, C.A. Petty. “Turbulent energy redistribution in spanwise rotating channel flows,” *Ind. Eng. Chem. Res.*, Special Issue, Stuart Churchill Festschrift, 50 (15), 8905–8916 (2011).

C.A. Petty, S. Muthu, K.S. Koppula, A. Bénard. “Interpenetrating continua and multiphase turbulence,” *Proceedings of 8th International Conference on CFD in Oil & Gas, Metallurgical and Process Industries*, SINTEF/NTNU, Trondheim, Norway (21–23 July 2011).

K.S. Koppula, A. Benard, C.A. Petty. “Realizable algebraic Reynolds stress closure,” *Chem. Eng. Sci.*, Special Issue, Morton Denn Festschrift, 64, 4611–4624 (2009).

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RESEARCH INTERESTS

Computational Materials Science, especially for Li ion batteries, oxide fuel cells, lightweight materials

LAB

Materials Simulation for Clean Energy (MSCE) Lab, 1260 & 3270 Engineering Building

WEBSITE

http://researchgroups.msu.edu/msce

SPECIAL EQUIPMENT AVAILABLE

Dedicated computer clusters at the MSU High Performance Computing Center

GROUP MEMBERS

Tridip Das, Christine James, Kwang Jin Kim, Yuxiao Lin, Jialin Liu, Hong-Kang Tian, Sanket Kadam, Dr. Yunsong Li

PATENT AWARDED

Y. Qi, J. Moote, Q. Lin, S. Harris , "Battery module for mitigating gas accumulation and methods thereof," US patents issued US9281548 B2. (3/2016).

RECENT ACHIEVEMENTS

TMS Brimacombe Medalist Award (2017).

MSU Strategic Partnership Grants on "de Novo Computational Methods for Simulating Energy Materials" (2016).

CURRENT RESEARCH

At the Materials Simulation for Clean Energy (MSCE) Lab, Qi and her group develop multi-scale simulation methods to design materials atom by atom. We are interested in materials that deliver clean energy. In the last several years, research grants from NSF, DOE, MSU, and GM allow the MSCE lab to study anode and cathode materials for lithium ion batteries, design brazing alloys for solid oxide fuel cells, and predict the role of oxides in aluminum casting.

Utilizing the high performance computer center (HPCC) at MSU and both commercial and homemade software, we are specialized at designing materials from their atomic structures. We screen materials chemistry with First-Principles methods, which solve the fundamental quantum mechanical equations of matter to calculate accurately the properties that are difficult to measure experimentally. We simulate materials behavior that involves millions of atoms using molecular dynamics with faster and accurate atomic interactions (force field). The multi-scale simulation tools we use and develop include: Density Functional Theory (DFT), Large Scale Molecular Dynamics, Reactive Force Field, Parallel computing, Phase field model, Mesodyn, Coarse Graining Schemes, COMSOL, and Finite Element Method. We have successfully integrated nano-scale insights learned from atomic simulations into meso- and micro- structures, governed by continuum theories, to design materials that are important for energy efficient and sustainable transportation industry. Central to these applications is a combination of "top-down" and "bottom-up" multi-scale modeling strategy with an associated experimental/ modeling research program. Therefore, most of our projects have strong collaboration with experimental groups and industry.

Currently, ongoing projects include:

Electron and ion transport in complex materials and interphases. Defect mediated diffusion greatly affects the power performance of battery and fuel cell devices. Using DFT informed thermodynamics formulation, we developed a systemic approach in 2015 to predict ionic conductivity as a function of voltage, pressure, temperature in single and polycrystals. In 2016, we extended our approach to include the more efficient density functional tight binding (DFTB) method, so that the transport properties of nano-meter thick solid electrolyte interphase (SEI) sandwiched at the electrode and electrolyte interface, a system with 1000 atoms, can be predicted with quantum accuracy. Currently, these methods were used to understand and design high energy density electrode materials for Li-ion batteries; solid electrolytes coating with fast Li ion transport, and cathode catalyst with large oxygen vacancies to reduce the operating temperature of solid oxide fuel cells.

Predicting chemical-mechanical degradation in Li-ion batteries. In order to computationally screen and design future battery materials for improved durability, we need to be able to predict failure starting from materials' properties and structures without using non-physical fitting parameters.

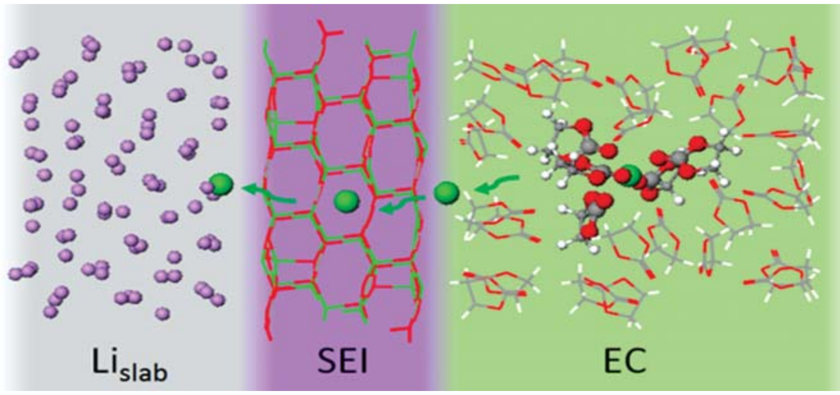

FIGURE 1. Density functional tight binding (DFTB) method along with the newly developed parameters is used to understadn lithium depletion and plating process, in the presence of a nanometer thick SEI layer. The work will lead to protective layer design on Li electrode for high energy battreies. *Accounts of Chemical Research* (2016).

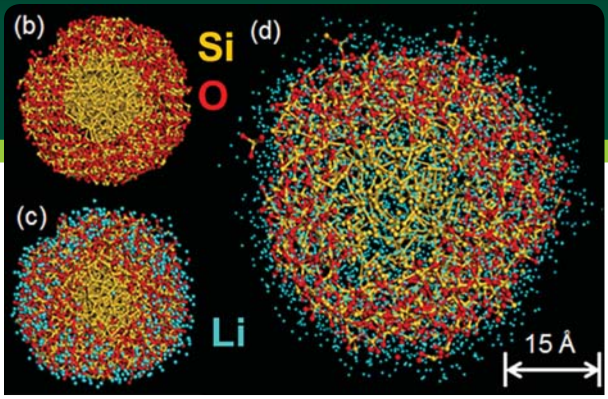

FIGURE 2. Simultaneously tracking and correlating the lithiation rate, compositional change, mechanical property evolution, stress distributions, and fracture of coated Si nanostructures at atomistic scale. *Phys. Chem. Chem. Phy.* (2016).

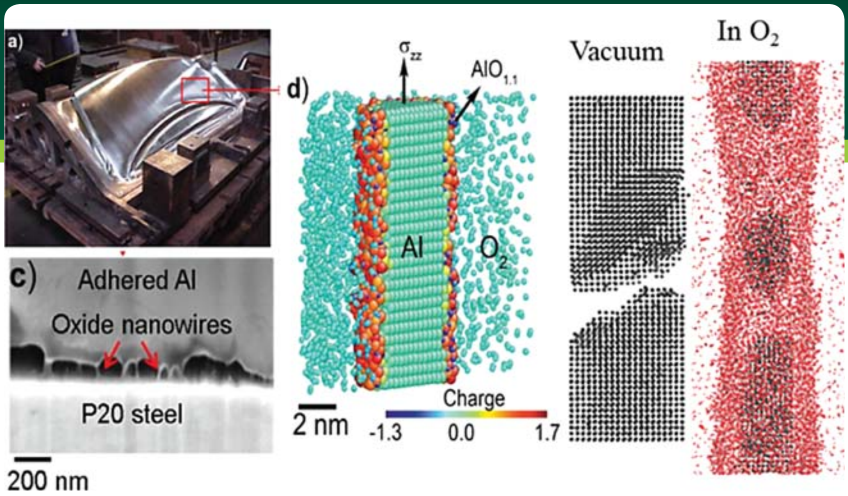

FIGURE 3. During hot-forming of Al-Mg alloy to make the lift gate of a car, nanowires were formed at adhered interfaces. Reactive molecular dynamics shows that Al nanowire deformation is drastically different in vacuum and O_2. *Nature Communication* (2014).

We have used DFT to predict the elastic and fracture properties of electrode materials and their interfaces, then integrated these properties into continuum model to predict the lithiation-induced stress and failure of composite electrodes. Many of our predictions have been confirmed by in-situ experiments. Currently, we are integrating structural evolution and chemical degradations into a battery predictive life model. We are using these methods to develop high capacity and long-lasting nano-structured electrodes.

The impact of environment on forming and machining light-weight materials. The environment (air, water, solution, electrolyte) can have a profound impact on deformation processes for light-weight metals (Al, Mg, Ta, Li, etc.) that have a high affinity to oxygen. Similar impacts of the environment are seen for electrode materials. By developing a reactive molecular dynamics method, we are able to track chemical reaction and mechanical deformation simultaneously and investigate their competing effect.

We have demonstrated how oxidation changes the deformation and failure mechanism in a nano-scale device, for example in an Al nano-wire. The nano-scale mechanisms also have a profound impact in large scale manufacturing processing, such as the tribology and surface quality of Al sheets for car panels made with hot forming processes. Currently, we are investigating the formation of a thin oxide layer on liquid aluminum during casting process and their influence on fatigue crack generation.

RECENT PUBLICATIONS

T. Das, J.D. Nicholas, Y. Qi, "Long-range charge transfer and oxygen vacancy interactions in strontium ferrite," *Journal of Materials Chemistry A* 2017, 5, 4493–4506.

F. Wang, Y.X. Lin, L. Suo, X. Fan, T. Gao, C. Yang, F. Han, Y. Qi, K. Xu, C.S. Wang, "Stabilizing high-voltage $LiCoO_2$ cathode in aqueous electrolyte with interphase-forming additive," *Energy and Environmental Science* 2016, 9, 3666–3673.

Y.S. Li, K. Leung, Y. Qi, "Computational exploration of the Li-electrode/electrolyte interface in the presence of a nanometer thick solid-electrolyte interphase (SEI) layer," *Accounts of Chemical Research* 2016, 49, 2363–2370.

Y.X. Lin, Z. Liu, K. Leung, L.Q. Chen, P. Lu, Y. Qi, "Connecting the irreversible capacity loss in Li ion batteries with the electronic insulating properties of solid electrolyte interphase (SEI) components," *Journal of Power Sources* 2016, 309, 221–230.

M.E. Stournara, R. Kumar, Y. Qi, B.W. Sheldon, "Ab initio diffuse-interface model for lithiated electrode interface evolution," *Phys. Rev. E* 2016, 94, 012802

C. James, Y. Wu, B.W. Sheldon, Y. Qi, "The impact of oxygen vacancies on lithium vacancy formation and diffusion in $Li_{2-x}MnO_{3-d}$," *Solid State Ionics* 2016, 289, 87–94.

J. Pan, Q. Zhang, X.C. Xiao, Y.T. Cheng, Y. Qi, "Design of nano-structured heterogeneous solid ionic coatings through a multi-scale defect model," *Applied Materials & Interfaces* 2016, 8, 5687–5693.

A. Ostadhossein, S.Y. Kim, E.D. Cubuk, Y. Qi, A.C.T. van Duin, "Atomic insight into the lithium storage and diffusion mechanism of SiO_2/Al_2O_3 electrodes of lithium ion batteries: ReaxFF reactive force field modeling," *The Journal of Physical Chemistry* A 2016, 120 (13), 2114–2127.

Q. Zhang, J. Pan, P. Lu, Z. Liu, M.W. Verbrugge, B.W. Sheldon, Y.T. Cheng, Y. Qi, X.C. Xiao, "Synergetic effects of inorganic components in solid electrolyte interphase on high cycle efficiency of lithium ion batteries." *Nano Letters* 2016, 16, 2011–2016.

Z. Liu, Y. Qi, Y.X. Lin, L. Chen, P. Lu, L.Q. Chen, "Interfacial study on solid electrolyte interphase at Li metal anode: implication for Li dendrite growth," *Journal of the Electrochemical Society* 2016, 163, A592–598.

S.Y. Kim, A. Ostadhossein, A.C.T. van Duin, X. Xiao, H. Gao, Y. Qi, "Self-generated concentration and modulus gradients coating design to protect Si nano-wire electrodes during lithiation," *Physical Chemistry Chemical Physics* 2016, 18, 3706–3715.

K.J. Kim, Y. Qi, "Vacancies in Si can improve the concentration dependent lithiation rate—molecular dynamics studies of lithiation dynamics of Si electrodes," *Journal of Physical Chemistry C* 2015, 119 (43), 24265–24275.

S. Patrick Walton

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RESEARCH INTERESTS

Biomolecular engineering and biotechnology

LAB

Applied Biomolecular Engineering Laboratory, 2125 Engineering Building

WEBSITE

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SPECIAL EQUIPMENT AVAILABLE

Fluorescent and chemiluminescent imaging, cell culture facilities

GROUP MEMBERS

Kevin Chen, Daniel Vocelle, Rebecca Carlson (UG), McKenna Coskie (UG), Calla Martysz (UG)

RECENT GRANTS

NSF–EHR–DUE "Supporting Excellent Engineers." AWARD #1643723; P.I.: Stephen Walton, CO-P.I.: Daina Briedis, Mark Urban-Lurain, Lisa Linnenbrink-Garcia, Theodore Caldwell, ORGANIZATION: Michigan State University, NSF ORGANIZATION: DUE, START DATE: 02/01/2017; AWARD AMOUNT :$1,000,000.

NSF–CBET. UNS: "Biomolecular Engineering of siRNAs." AWARD #1510895, P.I.: Stephen Walton, CO-P.I.: Christina Chan, ORGANIZATION: Michigan State University, CBET START DATE: 07/01/2015; AWARD AMOUNT: $350,000.

EAGER: "Biomanufacturing: CRISPR to increase the homogeneity and efficiency of stem cell differentiation." AWARD #1547518, P.I.: Christina Chan; CO-P.I.: Stephen Walton, ORGANIZATION:Michigan State University, CBET START DATE: 01/01/2016, AWARD AMOUNT: $263,584.

CURRENT RESEARCH

One achievable goal of the 21st century is "personalized medicine," the design of diagnostics and therapeutics specifically for a single patient. Reaching this goal depends on the development of new diagnostic approaches that can acquire vast quantities of data simultaneously, improving our understanding of the behavior of diseased cells, and therapeutics that can be delivered specifically to the diseased cells and can target the molecular-scale causes of the disease with exceptional activity and specificity.

The Applied Biomolecular Engineering Laboratory (ABEL), led by S. Patrick Walton, is currently working in both these areas, specifically on technologies that rely on nucleic acids (i.e., DNA and RNA). Areas of investigation include: (1) designing nucleic acid-based therapeutics based on understanding their mechanism of action and (2) applying genome editing to improve the understanding of cellular responses to stimuli. Recent work involves investigating how proteins interact with a new class of therapeutics, short, interfering RNAs, moving towards guidelines for designing these molecules. Additionally, the ABEL is applying CRISPR/Cas9 genome editing to manipulate stem cell responses to differentiation signals.

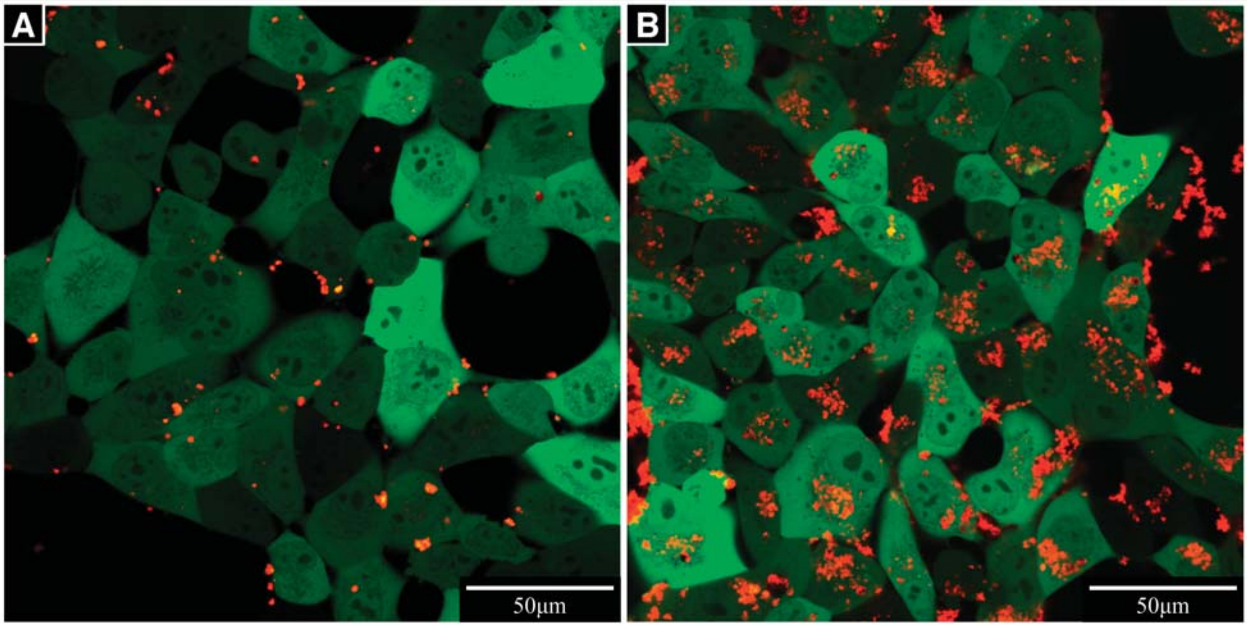

FIGURE 1. Confocal microscopy of delivery vehicle mediated silencing. Confocal images of cells (green) and fluorescently labeled siRNA (red) delivered by (A) a commercial reagent or (B) our nanoparticles.

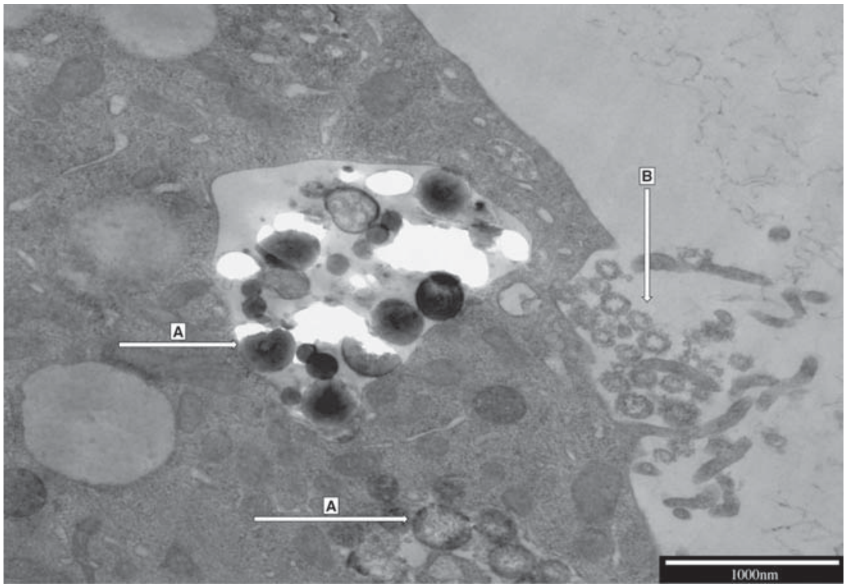

FIGURE 2. Microscopic analysis of nanoparticle-siRNA complex uptake and trafficking. Nanoparticles show intracellular degradation (A) and secretion (B).

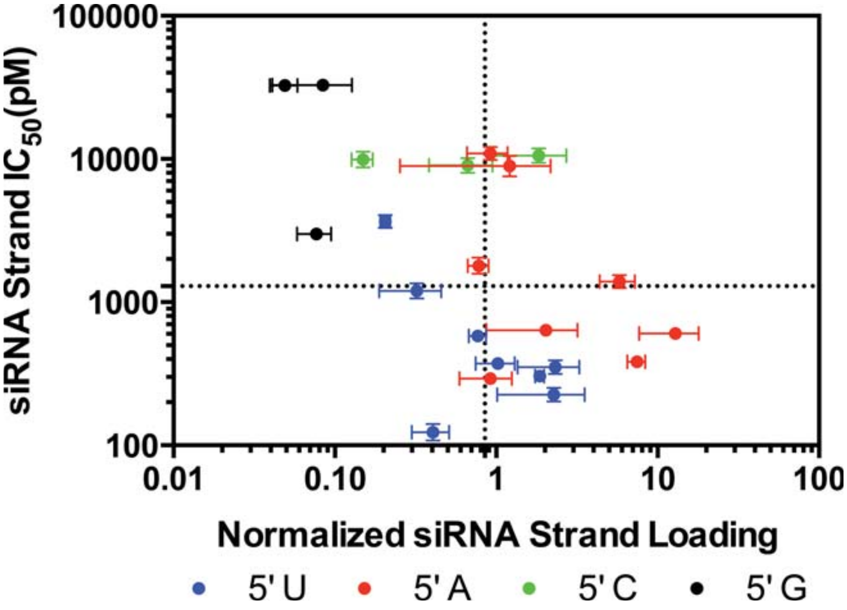

FIGURE 3. Correlation of single-stranded siRNA strand activity with loading. The imperfect correlation lets us design for each of these properties independently.

RECENT PUBLICATIONS

B. Bilgin, A. Nath, C. Chan, S.P. Walton, "Characterization of transcription factor response kinetics in parallel," *BMC Biotechnology* 16: 62 (2016).

P.A. Angart, R.J. Carlson, K. Adu-Berchie, S.P. Walton, "Terminal duplex stability and nucleotide identity differentially control siRNA loading and activity in RNA interference," *Nucleic Acid Therapeutics* 26(5): 309–317 (2016).

D. Vocelle, O. Chesniak, A. Malefyt, G. Comiskey, K. Adu-Berchie, M. Smith, C. Chan, S.P. Walton, "Dextran functionalization enhances nanoparticle-mediated siRNA delivery and silencing," *Technology* 4(1): 42–54 (2016).

D. Vocelle, C. Chan, S.P. Walton, "How can novel microscopic approaches shed light on the function of nucleic acid-based drugs?" *Future Med Chem.* 7(13): 1623–1625 (2015).

D.A. Lynam, D. Shahriari, K.J. Wolf, P.A. Angart, J. Koffler, M.H. Tuszynski, C. Chan, S.P. Walton, J. Sakamoto, "Brain derived neurotrophic factor release from layer-by-layer coated agarose nerve guidance scaffolds," *Acta Biomaterialia* 18: 128–131 (2015).

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RESEARCH INTERESTS
Biomolecular design and engineering

LAB
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WEBSITE
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GROUP MEMBERS
Matt Faber, Angelica Medina-Cucurella, Emily Wrenbeck, John Wright

RECENT ACHIEVEMENTS
Young Scientist Keynote, PEGS Meeting (2017)

PATENT
"Polypeptides for treating and/or limiting influenza infection," D. Baker, S.J. Fleishman, T.A. Whitehead. US Patent 9,181,300 (2015).

CURRENT RESEARCH
Engineering life is a broad-stated goal of the new generation of biological engineers. To better accomplish this goal, these engineers pursue the ability to design novel functions rather than rely on a catalog of "parts" culled from nature. Proteins, one of the main categories of parts, are wondrously complex biomolecules comprised of thousands of atoms, which fold into tertiary structures necessary for function by balancing competing inter- and intra-molecular forces. Imparting novel and specific functions into proteins is a difficult problem because protein structures are only marginally stable, protein structure-function relationships are not well understood, and many targeted small molecule substrates differ by as little as a single hydroxyl group or a methyl bond. The net result is that efforts to engineer or design new/improved proteins are either empirical in nature or suffer from low success rates, frustrating efforts to rationally and reliably redesign components for cellular life.

My group works to solve the problem of engineering proteins. We use and develop computational techniques to design proteins for new functions, have pioneered experimental approaches to comprehensively assess the effect of a protein's sequence on its desired function, and have imparted evolutionary and computational ideas to formulate efficient routes to optimize protein function. We are now interested in developing proteins for diverse applications like vaccine design and creating the next generation of biofuels. Our laboratory is funded by several State and Federal agencies, including the National Institutes of Health, the National Science Foundation, and the Department of Energy.

Recent highlights from the lab include:

Rapid conformational epitope mapping of antibodies. Antibodies that target specific antigenic epitopes on the surfaces of viral and bacterial pathogens can neutralize infection. Conformational epitopes, which exist when an antigenic protein is properly folded, are targeted by broadly neutralizing antibodies for a variety of pathogens like influenza and HIV. While obtaining the structural basis of how antibodies bind specific pathogens is key for the design of structure-based prophylactics, therapeutics, and vaccines, current methods for conformational epitope determination are low-throughput and laborious. My group has developed a fast, robust, and inexpensive method to map the conformational epitopes of antigens targeted by antibodies. This crucial missing link is being used in labs worldwide to expedite rational structure-based design of treatment and prevention options for a range of human pathogens.

RECENT PUBLICATIONS

E.E. Wrenbeck, M. Faber, T.A. Whitehead, "Deep sequencing methods for protein engineering and design," *Current Opinion in Structural Biology* 45:36–44 (2017).

C. Haarmeyer, M.D. Smith, S. Chundawat, D. Sammond, T.A. Whitehead, "Insights into cellulase-lignin non-specific binding revealed by computational redesign of the surface of green fluorescent protein," *Biotechnology & Bioengineering* (in press 2016)(doi:10.1002/bit.26201).

E.E. Wrenbeck, J.R. Klesmith, A. Adeniran, J.A. Stapleton, K.J. Tyo, T.A. Whitehead, "Plasmid-based single-pot saturation mutagenesis," *Nature Methods* 13(11): 928–930 (2016) (doi:10.1038/nmeth.4029).

J.R. Klesmith, J.P. Bacik, R. Michalczyk, T.A. Whitehead, "High-resolution sequence function mapping of a levoglucosan utilization pathway in *E. coli*," *ACS Synthetic Biology* 4 (11), 1235–1243 (2015) (doi: 10.1021/acssynbio.5b00131).

C.A. Kowalsky, M. Faber, A. Nath, H. Dann, V.W. Kelly, L. Liu, P. Shanker, E.K. Wagner, J. Maynard, C. Chan, T.A. Whitehead, "Rapid fine conformational epitope mapping using comprehensive mutagenesis and deep sequencing," *Journal of Biological Chemistry* 290 (44), 26457–26470 (2015) (doi:10.1074/jbc.M115.676635).

J.A. Stapleton, T.A. Whitehead, V. Nanda, "Computational redesign of the lipid-facing surface of the outer membrane protein OmpA," *PNAS* 112(31):9632–9637 (2015).

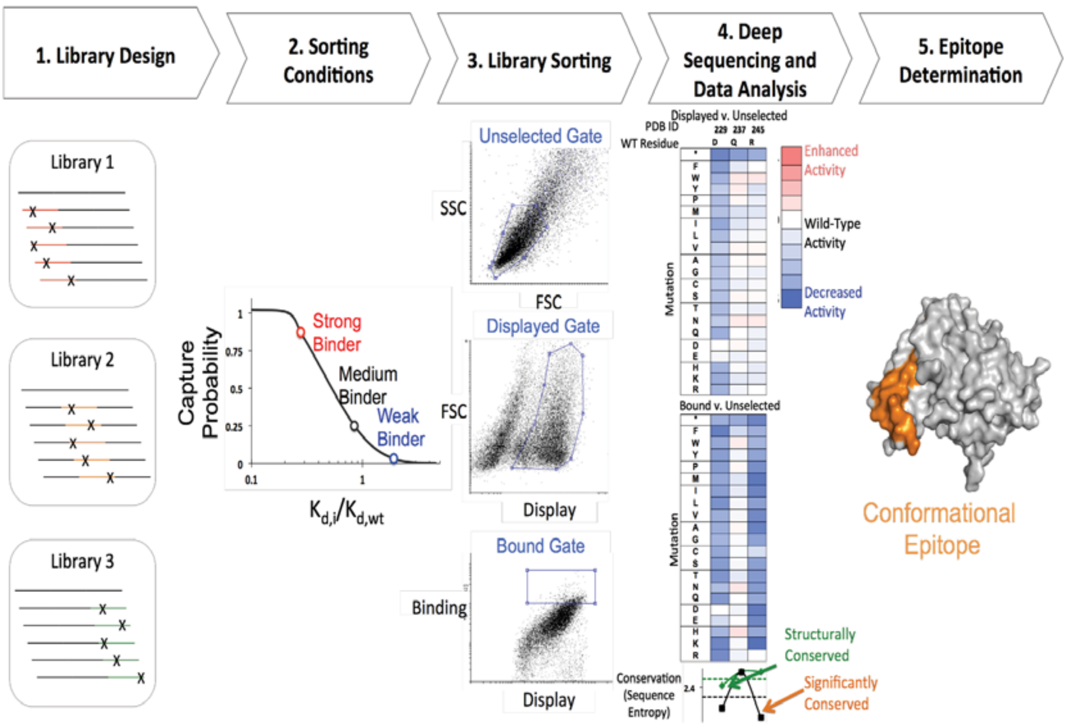
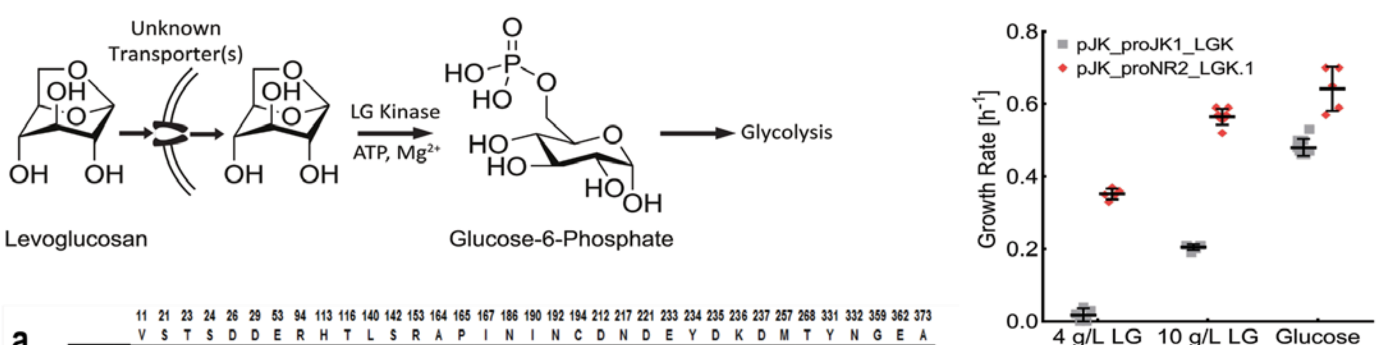


FIGURE 1: INNOVATION.

- We have developed a streamlined method to identify conformational epitopes for antibody-antigen interactions
- Can map epitopes for diverse enveloped viruses—improve diagnostics, suggest ways to design new/improved vaccines and therapeutics
- Method can be applied to enveloped viruses of interest to DTRA/Gates (Ebola, Rift valley fever, Marburg, Dengue, Newcastle Disease Virus, PPR, etc.)
- Future interests: Combining with computational design to develop novel protein-based vaccines



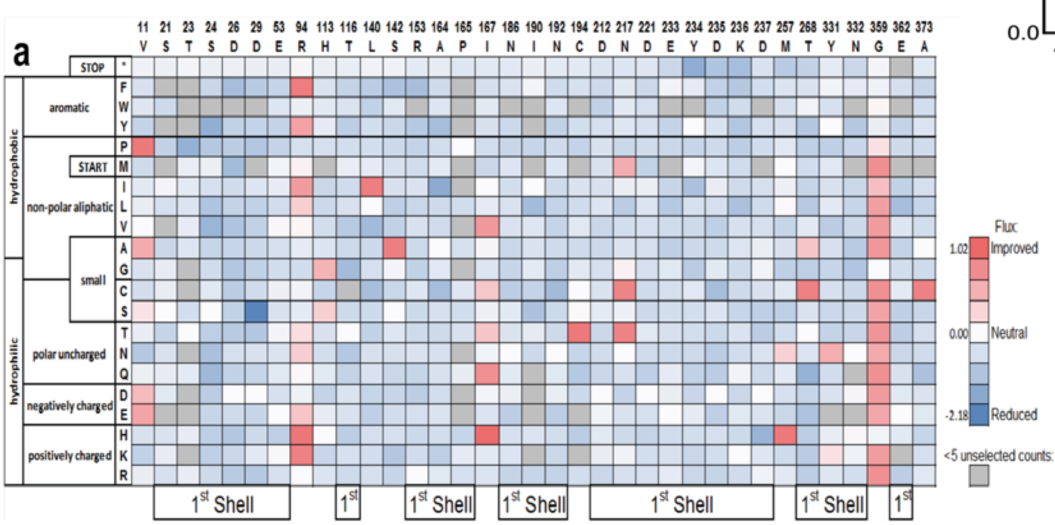


FIGURE 2: TRANSFERABILITY ACROSS FIELDS.

- We can use the same high-resolution method to optimize synthetic metabolic pathways

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RESEARCH INTERESTS

Multiphase biocatalysis, nanobiotechnology, biomimetic interfaces, biosensors, bioelectronics

LAB

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GROUP MEMBERS

Paul Sharpe, Neda Rafat, Serban Peteu

PATENTS

"Nanostructured biosensor containing neuropathy target esterase activity," US Patent 8,623,196 (1/7/2014).

"Customizable and renewable nanostructured interface for bioelectronic applications," US Patent 8,435,773 (5/7/2013).

"Microbial nanowire production." Provisional patent application, serial #61/558,091, submitted 11/10/2011; international application submitted 8/30/2012, entitled "Microbial nanowires and methods of making and using."

"Catalytic bioreactors and methods of using same." Provisional patent application, serial #61/531,304, submitted 9/6/2011; international application #PCT/US2012/053958 filed 9/6/2012, entitled "Catalytic bioreactors and methods of using same."

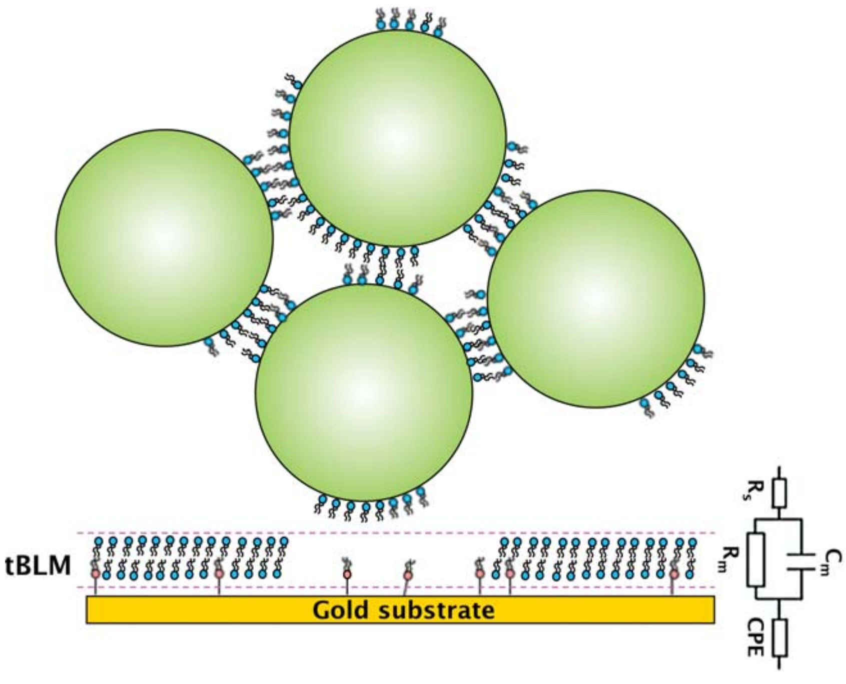

FIGURE 1. Schematic diagram of nanoparticles (spheres) removing lipid molecules from a biomembrane (shown as a layer of lipid molecules on the gold electrode).

CURRENT RESEARCH

Multiphase biocatalysis. Focus includes developing cost-effective and carbon-neutral methods to produce biofuels and chemicals from high-energy gases such as hydrogen and carbon monoxide. His group has been funded by the NSF and DOE to use microbubbles to enhance gas mass transfer. In a recent project funded by DOE's ARPA-E Electrofuels program, Dr. Worden's lab collaborated with the group of Dr. Anthony Sinskey at MIT to develop a bioprocess for continuous conversion of the gaseous reactants H_2, CO_2, and O_2 into the biofuel isobutanol (IBT). To address the three significant bioreactor-design challenges: (1) extremely high demands for gas mass transfer; (2) safety issues resulting from the simultaneous use of by H_2 and O_2 gases, which form explosive mixtures; and (3) biocatalyst inhibition by the IBT, Dr. Worden's group developed a novel Bioreactor for Incompatible Gases (BIG). The BIG features a hollow fiber module that allows the H_2 and O_2 gases to be kept on opposite sides of the membrane and transferred to the cells without forming unsafe gas mixtures. In addition, product inhibition is controlled by continuous removal of the IBT as it is formed. A prototype bench-scale BIG has been assembled in a walk-in hood, and an automatic process control system has allowed the bioreactor stably for up to 19 days. These experiments have demonstrated for the first time continuous IBT production from H_2, CO_2, and O_2.

Nanobiotechnology and biomimetic interfaces. This focus has recently been used to better understand cell toxicity caused by engineered nanomaterials (ENM). The approach uses an artificial bilayer lipid membrane (BLM) to mimic a cell membrane. When ENM interact with a BLM, pores are formed in the BLM, and the resulting leakage of ions through the pores can be measured. Dr. Worden's group recently used electrochemical impedance spectroscopy provides a sensitive method to measure ENM's potency in disrupting biomembranes. One study showed that the method could discern differences in the potency of polystyrene nanoparticles (PNP) having different in size and surface charge. Negatively charged, carboxyl modified PNP 20 nm in diameter were more potent in disrupting BLM than those 100 nm PNP. However, positively charged amidine modified nanoparticles, 120 nm PNP were more potent than 23 nm PNP.

Biosensors and bioelectronics. This focus is exemplified by a project funded by the NSF Accelerating Innovation Research program to advance a biosensor patent toward commercialization. The project addresses the need for more high-performance, inexpensive biosensors able to detect toxic organophosphorus pesticides and nerve agents. The objectives are (1) to adapt the redox-cycling biosensor interface to nanoparticle-functionalized electrodes, (2) to develop a redox-cycling biosensor interface for alkaline-phosphatase-linked antibodies, and (3) to adapt redox-cycling biosensor interfaces to three commercial biosensor platforms. Conductive nanomaterials are being incorporated into the bioelectronic sensor interface and functionalized to measure activity of a organophosphate as an electric current. Additional bioelectronic sensors are also being developed that use a redox-recycling mechanism to amplify biosensor signals that measure binding of enzyme-linked antibodies to their target antigen. A portfolio of potentially commercializable prototype bioelectronic immunosensors is being developed in collaboration with an original equipment manufacturer.

Dr. Worden has been active in leveraging research in these areas to develop novel educational programs that integrate multidisciplinary research with pedagogy. He has served as PI on two grants by the Department of Education's Graduate Assistance in Areas of National Need (GAANN) program to develop graduate Ph.D. training programs entitled, "Interdisciplinary Training Program on Bioelectronics" (seven co-Is) and "Multidisciplinary Graduate Training Program on Technologies for a Biobased Economy" (seven co-Is). He also served as PI of a grant from the NSF Combined Research and Curriculum Development program to develop a novel "Multidisciplinary Bioprocessing Laboratory" course (five co-PIs). He and a colleague from the Michigan Biotechnology Institute were funded by the US State Department to co-develop a fermentation scale-up training program for Russian bioscientists entitled "Fermentation Pilot-Plant Training for Sibbiopharm Staff."

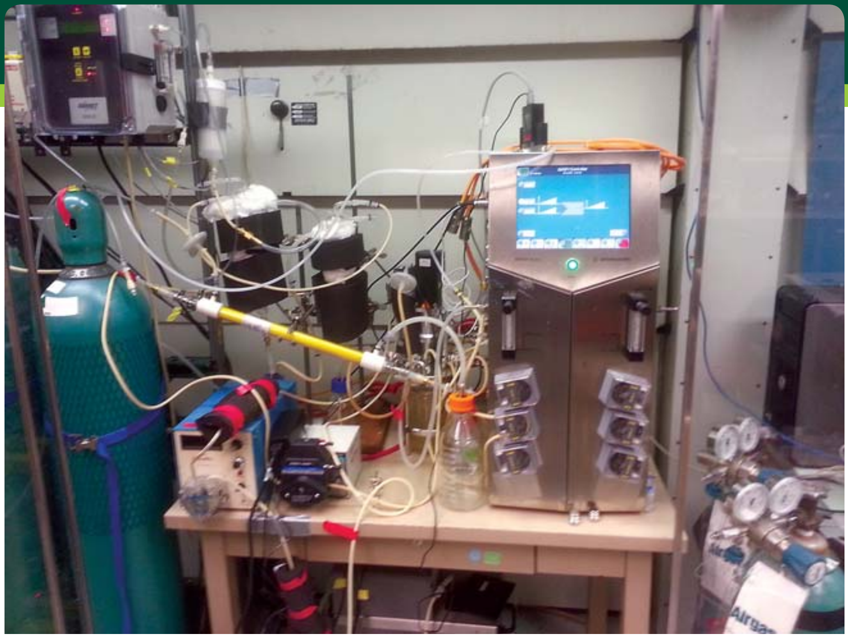

FIGURE 2. Photograph of prototype Bioreactor for Incompatible Gases (BIG) assembled in walk-in fume hood of Dr. Worden's laboratory.

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RESEARCH INTERESTS

Crystal growth; crystallography; thermal properties of materials, including thermal expansion, sound velocity, bond anharmonicity

LAB

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SPECIAL EQUIPMENT AVAILABLE

Optical floating zone furnace for crystal growth up to 2200°C; resonant ultrasound spectroscopy for measurement of elastic constants and sound velocity up to 500°C in controlled atmosphere; high-resolution, high-speed x-ray diffractometer with 2D pixel array detector, and high-temperature stage with controlled atmosphere up to 1400°C

GROUP MEMBERS

PHD STUDENTS: David Smiadak, Wanyue Peng. UNDERGRADS: Mack Marshall, Gill Levental.

CURRENT RESEARCH

Our research leverages crystal growth and high temperature characterization techniques to study the relationship between atomic structure, bonding and the electronic and thermal properties of functional materials. Ultimately, we aim to apply this understanding to engineer improved functional materials for energy applications. Our recent efforts have focused on optical floating zone growth of single crystals and measurements of the high-temperature sound velocity and lattice expansion in materials used for thermoelectric energy conversion.

Crystal growth of anistropic materials. Our current aim is to develop improved thermoelectric materials for use in radioisotope thermoelectric generators designed and tested at NASA's Jet Propulsion Laboratory. The thermoelectric materials used in this application must be semiconductors with very high melting temperatures, optimized electronic properties, and low thermal conductivity. They must also be mechanically robust over a large temperature gradient.

Many candidate materials have atomic structures that are extremely anisotropic, and are therefore predicted to have more favorable electronic properties along specific crystal orientations, as illustrated in Figure 1 for $Ca_5Al_2Sb_6$. This anisotropy is expected to lead to improved thermoelectric properties along the high conductivity direction. One of the most significant barriers, however, to understanding the intrinsic electronic and thermal properties of complex semiconductors is the scarcity of large single crystal samples. This is particularly limiting in the case of anisotropic materials, for which measurements of bulk, single crystalline samples yield only "averaged" properties.

In our laboratory, we are utilizing several high-temperature techniques to grow single crystals of semiconducting and ceramic materials from the melt. Our main focus is optical floating zone growth, illustrated in Figure 2, which is a powerful method for materials with very high melting temperatures and relatively low vapor pressures. An optical floating zone furnace consists of several halogen lamps set in elliptical mirrors (four, in our case). The mirrors focus the light on the center of the chamber, where two polycrystalline rod-shaped samples are suspended inside of an inert gas-filled quartz tube. A stable

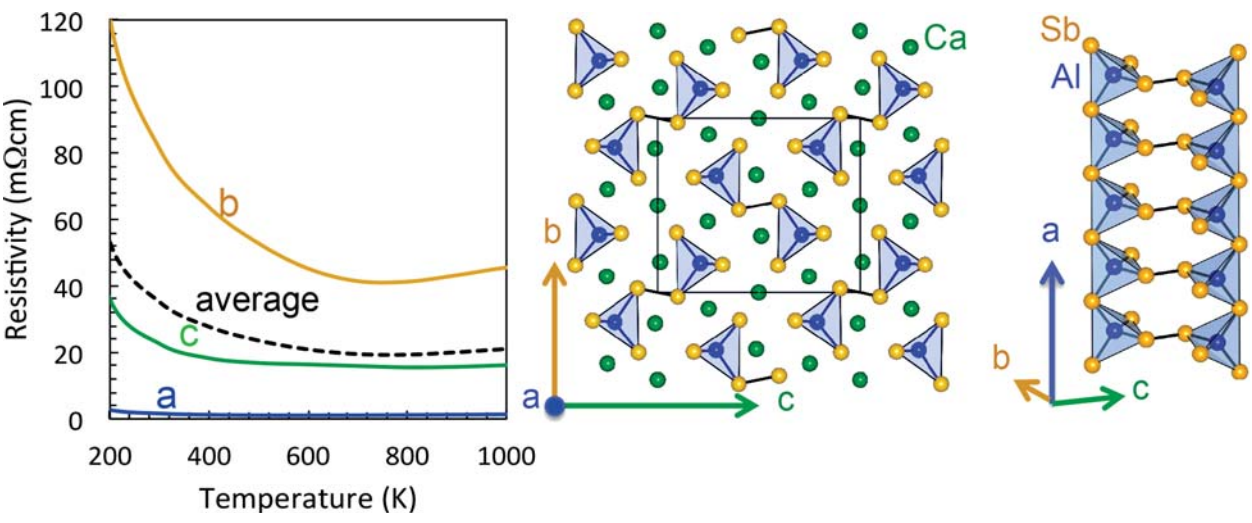

FIGURE 1. The predicted electronic properties of $Ca_5Al_2Sb_6$, a thermoelectric material with a complex crystal structure, are predicted to be highly anisotropic. $Ca_5Al_2Sb_6$ single crystals are necessary to prove this experimentally.

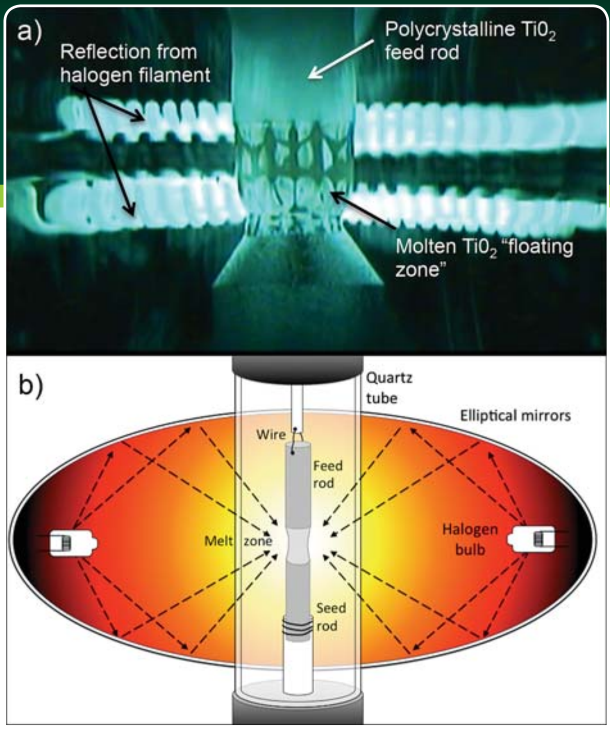

FIGURE 2. (A) Screenshot from the growth of a TiO_2 crystal using the optical floating zone method. (B) Schematic of the interior of a floating zone furnace showing the sample mounted inside of an evacuated quartz tube. Light from four halogen bulbs is focused on the center of the sample, creating a floating molten zone.

"floating" molten zone is established where the two rods meet. During growth, both rods are moved downwards, so that the floating zone slowly progresses up the length of the feed rod. This method can also be adapted to materials with incongruent melting behavior by employing a molten flux (i.e., solvent material) instead of melting the target compound.

Resonant Ultrasound Spectroscopy. The thermal and elastic properties of materials are critical in a wide range of applications. Resonant ultrasound spectroscopy (RUS) is an elegant approach to characterize the elastic constants of bulk and single crystal samples by measuring the vibrational resonant frequencies.

RUS uses a drive transducer to sweep across a range of frequencies and a pick-up transducer to record the response. The resonant frequencies are a function of the elastic constants, sample geometry, and sample density. This method is also ideal for measuring the full elastic tensor of anisotropic single crystals, as the entire tensor is obtained in a single measurement. High temperature RUS measurements coupled with high temperature x-ray diffraction—also available in our laboratory—gives us an extremely sensitive set of tools to investigate structural changes in materials, including gradual softening of bonds, order-disorder transitions, and structural phase changes.

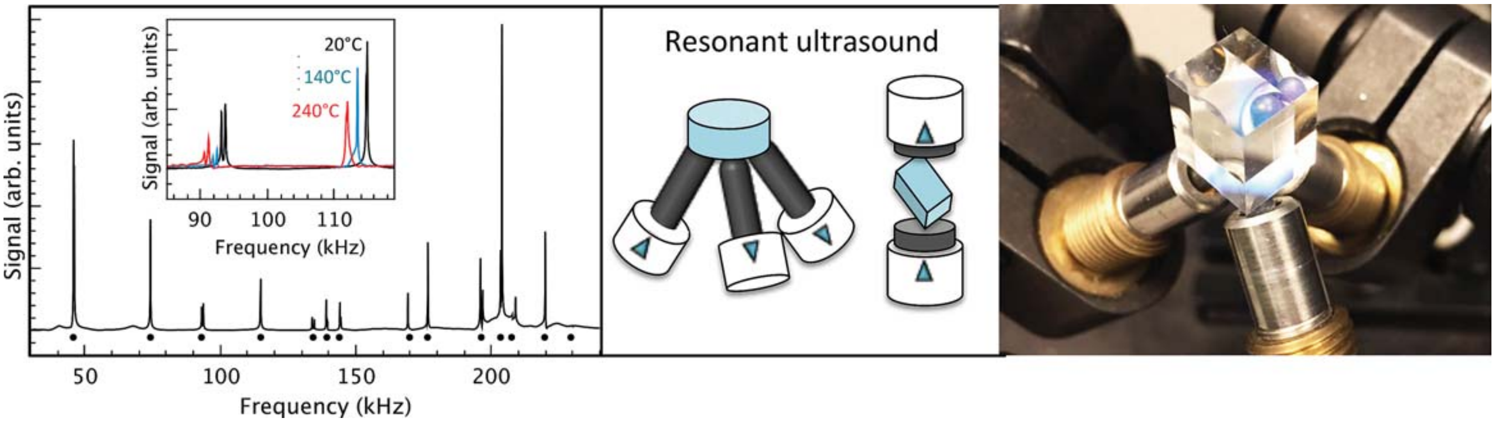

FIGURE 3. The resonant ultrasound method uses a piezoelectric transducer to emit acoustic waves over a range of frequencies. Certain frequencies will resonate strongly in the sample, yielding a vibrational response that is detected by a second transducer. This method allows us to study the elastic tensor of single crystals and polycrystalline materials at room temperature and at high temperatures.

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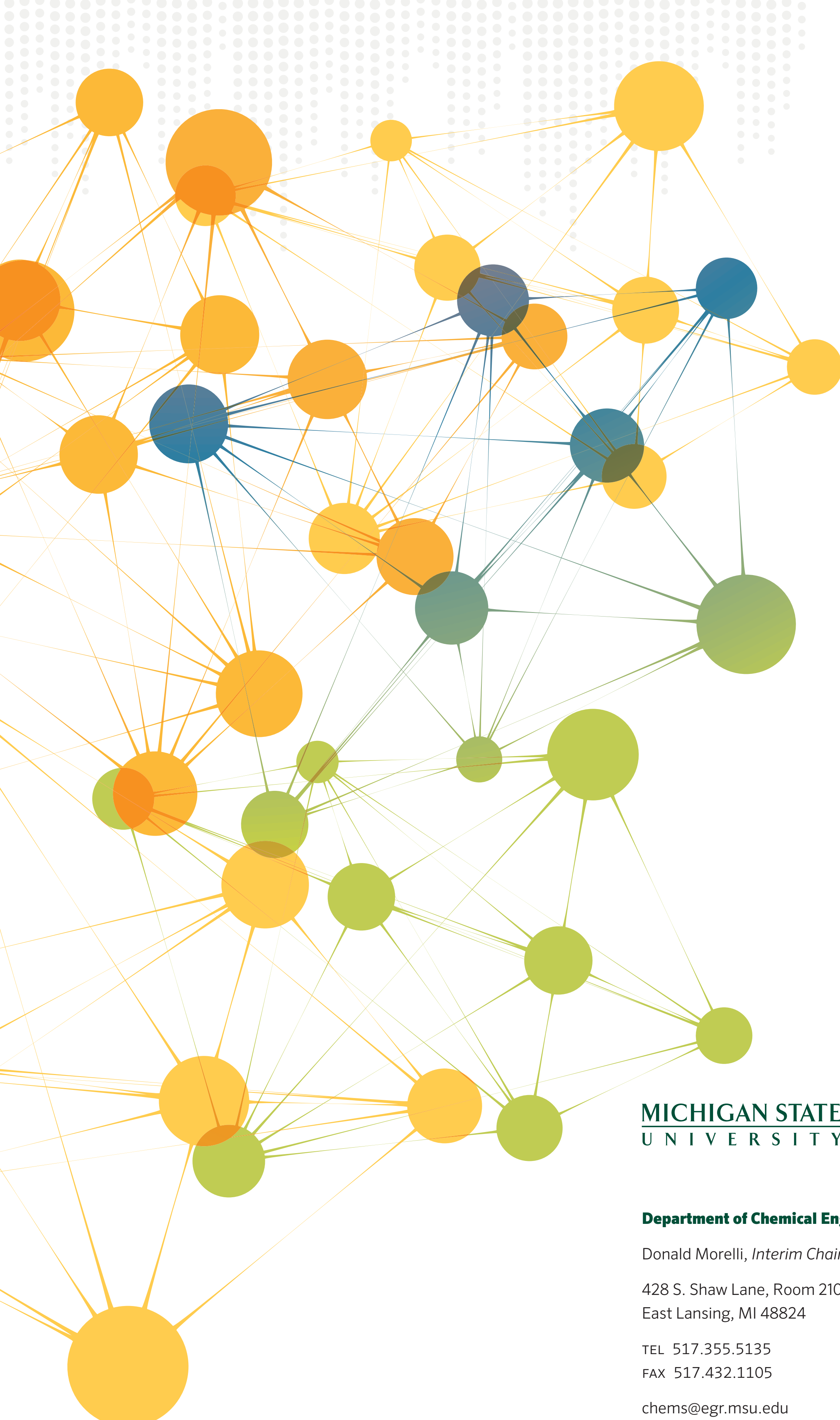

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