Orientation map of a stainless steel sample produced by direct melt laser sintering additive manufacturing. The data were collected by electron backscatter diffraction analysis.
Dear Alumni and Friends,

Greetings from the School of Materials Science and Engineering (MSE) at Georgia Tech! I am delighted to share the highlights and events that shaped this past year. Our enrollment peaked to approximately 390 undergraduate and 185 graduate students. We welcomed two new faculty, Natalie Stingelin from Imperial College in London, and Blair Brettmann from the University of Chicago, which further strengthens our soft/bio and functional materials research groups.

We initiated the new graduate curriculum with all students entering the MSE Ph.D. program taking a common core of two courses (Thermodynamics and Structure of Materials) followed by the flexibility of taking the remaining courses in any area. The MSE “maker and measure” space, The MILL—Materials Innovation and Learning Laboratory—is now equipped with 3D printers, filament extruders, and furnaces for materials processing, benchtop SEM, XRD, and FTIR for structure characterization, tensile and hardness testers, DMA, fiber-optic UV/vis, and micro viscometer for property measurement. We thank Art and Patricia Cox, the 3M Foundation, and Georgia Tech Technology Fee funds for the generous support that helped acquire the equipment. The capstone design teams continue to marvel our sponsors, and it is impressive to see the excellence of the work of our undergraduate (freshmen) scholars during their 10-week summer research activities. Entrepreneurship is pervasive among our students who are participating in CREATE-X and Ti:GER programs. This year, two of our Ph.D. graduates, Christopher Oberste and Matt Smith, started working for their own start-ups.

We were all proud to see our faculty and staff recognized during the annual Georgia Tech honors day event this year. They include Seung Soon Jang (Senior Faculty Outstanding Undergraduate Mentor Award), Zhiqun Lin (Sigma Xi Best Faculty Paper Award), Mark Losego (CTL/BP Junior Faculty Teaching Excellence Award), Mary Lynn Realff (CoE and ANAK Society Faculty Advisor Award), and Rusty Edwards, our revered assistant director for financial operations (Outstanding Achievement in Research Enterprise Enhancement Award). John Reynolds was elected Fellow of MRS and of the Royal Society of Chemistry.

It was with mixed emotions that we said good-bye to Dean Gary May, as he left Georgia Tech to be Chancellor of the University of California at Davis. Steven M. McLaughlin, the Steve Chaddick Chair and professor in the School of Electrical and Computer Engineering, has been appointed the new dean of our College of Engineering and Southern Company Chair. We look forward to working with Dean McLaughlin in the pursuit of excellence of our School and the College. With MSE as the hub of materials-related education and research at Georgia Tech, we are building interdisciplinary collaborations with faculty in various units and GTRI to address “big” ideas in research and learning by our students.

During the past year, I had the good fortune of visiting with many of our alumni working in academic institutions, industry settings, and national laboratories. Their recognition of the value of a Georgia Tech education, their words of wisdom, and the joy and enthusiasm they see in their current working environment, combined with their accomplishments, is a testament to the pride of a helluva engineer.

I feel privileged to have been at Georgia Tech for the past 25 years, and honored to have the opportunity to serve as the chair of MSE for the past five years. I am looking forward to working with our faculty, staff, and students, as we propel toward the next in academic and research excellence. I welcome you to come and visit us during your travels through Atlanta. Thank you for your continued support of the School and for all you do to help us make MSE at Georgia Tech an exceptional program.

Naresh Thadhani
Professor and Chair,
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After almost 12 years as director of development in the School of Materials Science & Engineering, I continue to be astounded by the creativity and talent of both our faculty and students. The visions and dreams of these incredible people are becoming realities daily, and I can picture a better future from their work. This is not only exciting, but also uplifting.

I am also profoundly impacted by the generosity of so many people: alumni, corporate and foundational representatives. The gifts we receive are as varied as the people who give them. Some are smaller, some larger, and they come in many forms—time, talent, and treasure—what we call the three Ts.

This energy, talent, and progress in MSE is what drives me to do what I do as a fund raiser. It's what drives me to pick up the phone to make those calls to people I don't know.

I'm inspired by the people who are so generous, with whom I get to work so closely. For those who have the capacity, I've discovered that loyalty and involvement often translates into philanthropy, regardless of giving ability. It's been gratifying over the years to get to know students and then see them staying involved with the School after graduation.

I am often asked what it's like to be post-campaign. The biggest difference is the opportunity to focus more on meeting new people and connecting them back to MSE.

I look forward to the future opportunities to share with you our new MSE stories of hard work, new paths, innovations, and novel solutions.

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Front cover: unpublished work by Josh Kacher and Jordan Key
New Hires

Keia Dodd

Keia Dodd joins MSE as a faculty support coordinator providing assistance for faculty within the Molecular Science and Engineering (MoSE) building. Keia first came to Georgia Tech in 2012, working for the School of Physics and the Enterprise Innovation Institute (EI²), respectively. She has previous experience working in the areas of administrative support, finance, and human resources.

Keia earned her bachelor's degree in sociology from Mercer University and is pursuing her Master's degree in Higher Education Administration from Georgia Southern University.

Nadia Barr

Nadia Barr, came to MSE as a financial administrative professional with several years of experience working in academia. For the past four years, she was an accountant with Georgia State University where she served as a lead staff member overseeing the departmental finances and personnel actions.

Nadia obtained her bachelor's degree in psychology from Georgia State University in 2011. After discovering a love for finance and working with many influential entrepreneurs, she completed her MBA with a concentration in finance from the University of West Georgia in 2016.

Roderick Ray

Roderick Ray is the new MSE financial administrator. For the past year, Roderick served as a staff accountant for the Meredith Corporation in Atlanta. In this role, he played a vital part in the month-end closing process, managing invoices, and communicating with various levels of management.

Roderick received his Bachelor of Science in Finance from Jacksonville State University in Jacksonville, Alabama. He is a diligent, adaptive, and intuitive recent graduate who is eager to continue growing in his professional career.

Good Byes

Angie Beggs

Angie Beggs retired after more than 30 years of dedicated service to Georgia Tech. Angie began her Tech career in 1976, but after a few years, left for “greener pastures.” In 1994, she returned after realizing that Tech was pretty green after all. She served in PTFE (which merged with MSE in July 2010), where she remained until she retired. She was an administrative manager for the last several years of her tenure. Angie’s service and commitment to both PTFE’s and MSE’s faculty, staff and students, as well as the GT community are truly noteworthy and will not soon be forgotten.

In her retirement, Angie is enjoying travel, community service work, scrap booking, and spending time with her family.

Linda Roberson

Longtime MSE employee Linda Roberson retired in June after more than 31 years of dedicated service to Georgia Tech. Linda began her career at Tech in 1981 as a receivable accountant in the bookstore. After a break in service from1983-1988, she returned to Tech, working in ECE, processing sponsored reporting for the Star Wars project. In 1992, she transferred to Polymer Textile Fiber Engineering (PTFE), where she spent 18 years. Upon the PTFE–MSE merger in 2010, Linda worked in finance until her retirement.

Linda's dedication and contribution to MSE will be greatly missed.
Accolades

**Young Investigator Faculty Awards**

- **Josh Kacher**, MSE, and **Wenshan Cai**, ECE with a joint appointment in MSE, both received the Office of Naval Research Young Investigator Award. This award is given to scientists whose research holds strong promise across several naval-relevant science and technology areas. Cai and Kacher were two of the 33 recipients selected from over 360 highly qualified applicants. Kacher was also awarded the DoE Basic Energy Science Early Career Award which supports the development of individual research programs of outstanding scientists early in their careers and stimulates research careers in the disciplines supported by the DOE Office of Science.

- **Mark Losego**

- **Matt McDowell**, ME with joint appointment in MSE, received the NSF Career Award for his research on interfacial transformations in ceramic ion conductors for solid-state batteries. McDowell also received the Air Force Office of Scientific Research Young Investigator Award and American Chemical Society Petroleum Research Fund Doctoral New Investigator Award.

- **The 2017 3M Non-tenured Faculty Award went to Mark Losego.** Presented by 3M's Research and Development Community in partnership with 3Mgives, the award recognizes outstanding new faculty who excel in research, experience, and academic leadership.

**Five MSE Students Receive Prestigious Fellowships**

MSE students Elizabeth Quigley, Emily McGuinness, Michelle Krecker, and Eric Hoar have been awarded the prestigious NSF Graduate Research Fellowship. The fellowship recognizes and supports outstanding graduate students in NSF-supported science, technology, engineering, and mathematics disciplines who are pursuing research-based graduate degrees at accredited United States institutions.

Emily McGuinness also received the National Defense Science & Engineering Graduate Fellowship (NDSEG). Abigail Advincula was another recipient of the NDSEG fellowship. The NDSEG is a highly competitive, portable fellowship designed to increase the number of U.S. citizens trained in disciplines of science and engineering important to defense goals. It is given to individuals who have demonstrated the ability and special aptitude for advanced training in science and engineering.

- **Elizabeth Quigley**
- **Emily McGuinness**
- **Michelle Krecker**
- **Eric Hoar**
- **Abigail Advincula**

**Nicole Kennard Receives Fulbright Fellowship**

Undergraduate student Nicole Kennard was selected to receive the prestigious Fulbright Fellowship. Nicole is pursuing a MSc in Sustainable Agriculture and Food Security and will be attending graduate school at Newcastle University in the U.K.

During her senior year, Nicole also received the MSE Outstanding Senior Award and was on the Faculty Honor's list.
Collaboration is the key to the future

“Science improves lives: each day we’re building, growing and working together to push the boundaries of innovation.” 3M website

Many companies throw out tag lines, but with 3M, it isn’t just a catchy phrase—it is a core belief by which the company, and its people, live. At Georgia Tech, and within the School of Materials Science and Engineering, we share these values and act on them every day.

The partnership between 3M and Georgia Tech reaches back to the 1970s, and over the years it has not only continued, but has grown considerably. We are so fortunate that today 3M provides support across the Institute, with a focus on students and young faculty.

Here in MSE, our strong relationship with 3M is, in large part, thanks to MSE alumnus, Geoffrey Morris (CerE ’82), 3M Oral Care, Scientific Affairs Manager, and current member of the MSE External Advisory Board. Through the years he has worked hard to promote Georgia Tech and MSE to 3M, and has been an active mentor to MSE students.

3M’s generous gift in support of the MILL, the MSE maker and measure space, enabled us to purchase five 3D printers, thus putting the “make” into the maker and measure space. Open to all students across campus, the MILL complements the renowned Invention Studio, connecting students at all levels with the tools and resources needed to encourage hands-on, active learning.

In 2015, MSE was the first recipient of a 3M Graduate Fellowship on the Georgia Tech campus. The honor went to Ph.D. student Alex Lohse, who spent this past summer at the 3M facility in St. Paul working on a method to monitor photopolymerization kinetics via in-situ NMR spectroscopy. Lohse enthusiastically describes the benefits of his fellowship: “From an R&D perspective, the 3M campus in St. Paul is truly remarkable. The company’s encouragement to test new ideas and the ability to collaborate with engineers and scientists at the top of their fields leads to some impressive technology in a wide range of industries from dental implants to office supplies.”

3M also recognizes the importance of helping young non-tenured faculty to achieve their goals in research and their careers. In 2011, Valeria Milam was the first MSE faculty to receive the 3M Non-Tenured Faculty Award. Dong Qin received the award in 2015, and Mark Losego in 2017. Zhiqun Lin received the award in 2006 when he was at Iowa State University.

In addition to providing funds for equipment and support for faculty and graduate students, 3M continues to sponsor and mentor MSE Undergraduate Research Scholars and Capstone Design projects at Georgia Tech.

As an institution, Georgia Tech’s primary job is to educate our students so they leave with a skill set that will allow them not only to have successful careers, but also a positive impact on our society, ultimately leaving the world a better place. 3M understands this and has a vision for the future of technology, innovation, and the people who will lead the way.

It is hard to put into words how grateful we are to 3M for their continued support of MSE and Georgia Tech. Perhaps the best way to demonstrate our appreciation is to continue to lead the way in innovation—in research, in teaching, and in program development—in partnership with their core values of collaboration and pushing the boundaries of innovation.
In Memoriam, Malcolm B. Polk

Malcolm B. Polk, 79, Professor Emeritus in the School of Materials Science and Engineering, died Monday, May 22, from complications arising from an operation.

Polk studied chemistry at the University of Illinois and University of Pennsylvania, followed by employment as a research chemist in the Plastics Division of the E. I. DuPont Co., Experimental Station. He left industry to join the chemistry department at Atlanta University in 1973. After joint collaborations with the faculty at Georgia Tech, Polk joined the then-School of Textile Engineering in 1985 as the first African-American professor in the School’s 88-year history.

Polk’s research interests included the synthesis of liquid crystalline polymers with unusual structures. His research program was fruitful, resulting in a series of internationally recognized journal papers and world-class graduates from his group. Polk was instrumental in developing the curricula for the new degrees in the Polymer, Textile, and Fiber Engineering Program in 2002, ensuring that the polymer content was incorporated at the highest level and rigor. He was known as a collegial partner to his colleagues and a beloved teacher to the students in his classes and research groups.

2016 Brumley D. Pritchett Lecture

John A. Rogers, Louis Simpson and Kimberly Querrey Professor of Materials Science and Engineering, Biomedical Engineering, and Neurological Surgery (and by courtesy Electrical Engineering and Computer Science, Mechanical Engineering, and Chemistry) at Northwestern University, presented the 2016 Brumley D. Pritchett Lecture. His presentation was entitled “Electronics for the Human Body.” The Pritchett Lecture Series is an annual event established in 2006 as a memorial to the late Col. Brumley D. Pritchett.

2017 CoE Alumni Awards

Spring Beasley, B.S. MSE ’92, M.S. EMIL-SCS ’15, Director and Chief Engineer of Payloads Engineering, Boeing Commercial Airplanes, received the Academy of Distinguished Engineering Alumni award. Beasley serves on the MSE External Advisory Board, the Women in Engineering Advisory Board, and is a mentor at Boeing, Georgia Tech, and several Seattle high schools. She is also a mentor/coach for Washington FIRST robotics Team Reign (the only all-girls robotics team in the tri-state area).

Kristen H. Brosnan, B.S. MSE ’99, Technical Operations Leader, Metals Discipline, GE Global Research, received the Council of Outstanding Young Engineering Alumni award. Brosnan is a featured science blogger for the GE Global Research external website and co-leader of the GE Women’s Network NY Capital District Hub, which aims to attract, develop, and retain women at GE. She is a mentor for student leaders in the American Ceramics Society, an advocate for diversity in the STEM professions, and a leader in STEM outreach to young women.
The Materials Innovation and Learning Laboratory (The MILL), the maker and measure space for the School of Materials Science and Engineering at Georgia Tech, opened its doors for student access in spring 2017. Students from throughout the Institute now have the opportunity to be trained by their peers in electron microscopy, compositional analysis, and multi-material 3D printing. While many engineering and science students have shown up at The MILL, these facilities have been most used by our students in MSE 2021 (materials characterization) and MSE 4420 (senior design) courses. The winning MSE senior design team, “Team Designers,” extensively used The MILL’s tabletop SEM to discover the source of thermomechanical wear in Under Armour uniforms designed for hard court sports.

Generous internal and external support has allowed The MILL to expand and include infrared and UV/vis spectroscopy, mechanical testing, glass and ceramic processing, and polymer extrusion for making custom filaments for 3D printing. The MILL’s staff has expanded to more than 20 students and expects further growth in the fall semester, with the goal of being open for 30+ hours per week. To further engage students in The MILL’s facilities, mini research projects are being developed in conjunction with faculty to explore the process-structure-property relations among various material classes. Student teams working on these research projects will present and compete for prizes at next year’s annual MSE spring poster session.

"My experience in the MILL has enriched my learning and has made me a more competent engineer. The MILL has significantly enhanced my education and has allowed me to holistically apply all of the knowledge I am learning in the classroom."

Shawn Gregory, MSE ’17

Looking Ahead to The MILL Year Two: Growth and Expansion

Josh Morton operating a 3D printer to demonstrate multi-material fabrication capability.

Shawn Gregory prepares samples for electron microscopy.
Summer 2017

MSE Research Scholars receive a $6000 stipend for 10-week immersion in summer research following completion of freshman year. They are encouraged to present their research at the annual fall MSE Industry Day event and to participate in the spring MSE poster competition. Summer 2017 industry sponsors included Kolon, Novelis, and Solvay.

Justin Chu, Deformation mechanism effects on fracture toughness of thin tin alloy sheets

Meha Kumar, Quantitative characterization of microstructures of AHSS steels

Zach Lowe, Nuclear forensics

Riddhi Patel, Production of nanofiber-particle composites using electrospinning

Chase Scott, Investigating the relationship between corrosion and microstructure in aluminum alloys

Laurel Stafani, Identifying oligonucleotide ligands for antimicrobial agents

Sanika Subhash, Using laser interactions with carbon nanoparticles to study drug delivery in cells

Punith Upadhya, Compositional and structural behaviors of Li halide hydroxides for their ionic conductivities

Sam Williams, Functional characterization of PZT, Mn-doped PZT, PMN-PT, and hetero-layers of PZT and PMN-PT

David Yeh, Engineering materials for solid-state energy storage systems

Ben Zusmann, Synthesis of nanowires of precious metals by chemical de-alloying

Tom Hodge, Ph.D. ChE ’96, Director of Materials Research, Michelin Americas Research Company

Tami Mace, MS Poly ’03, Materials Scientist, Program Leader, Surgical R&D, EcoLab Inc.

Sandra H. Magnus, Ph.D. CerE ’96, President, The American Institute of Aeronautics and Astronautics

Graeme Marshall, Director Global R&T Center, Global Technology Director, Enabling Science, Novelis Global Research & Technology Center

Angela Mitchell, PTCh ’04, Senior Engineer, R&D, Halyard Health

Geoffrey P. Morris, PE, CerE ’82, Materials/3M Oral Care, Scientific Affairs Manager, 3M

Yancy W. Riddle, M.S. MSE ’98, Ph.D. MSE ’01, SVP Operations, Nearshore Technology & Engineering

Herb Upton, Mgt. ’93, Director, Specialty Products Division, Shaw Industries Group

Phil Williams, EAB Vice Chair, Text ’70, Consultant

Emeritus Members

Jennifer P. Bailey, CerE ’70, M.S. CerE ’71, BASF (Retired)

Lee Bryan, Global Director of Product Supply, TenCate Geosynthetics

David Bowden, M.S. Met ’78, Ph.D. Chem ’82, Technical Fellow, Boeing Company (Retired)

Michael L. Fulbright, Text ’72, President and CEO (Retired), JPS Industries, Inc.

Michael Ginn, M.S. CerE ’80, President, Ginn Mineral Technology, Inc.


Jeffrey A. Martin, TE ’82, President and CEO, Yulex Corporation

Sponsor a MSE Research Scholar
Contact Mary Z. McEneaney, mary.mceneaney@mse.gatech.edu

Former research scholar Yungton (Cherry) Zhu discusses her research with Professor Seung Soon Jang.
Ryan Dwyer of Team Designers, 2017 MSE Capstone winner, discusses their project on Thermomechanical Failure of Hard Court Uniforms

3M, Synthetic Dentin
Team eeth - Philip Anschutz, Kinsey Canova, Onyeka Dimkpah, Kevin Fan, Erin Flynn, Hirsh Patel

Center for Disease Control, Building a Better Bed Net
Team Buzzkill - Alex Hamad, Nathan James, Bilal Khan, Hunter Ray, Mary Cate Robish, Ashanti Turner

Georgia Department of Transportation, Design and Conformation Specification for Concrete
Team Avalon - Abhinav Bhardway, James Christopher, Candace Ogata, Annie Song, Kevin Zhu

GT, SECure Bandage
Team Eclectic Shock - Kaustav Das (ME), Erin Fitzpatrick (BME), Brandon Holt (BME), Jack Jacoby (ME), Jun Ki Kim (MSE), Chenlu Li (ME)

GT, Flexible electronic moisture sensor for diapers
Team Flex Detect - Juan Navarrete (BME), Taylor Payne (ME), Vanessa Prema (MSE), Numera Sachwani (BME), Meghan Styles (BME), A’isha Williams (MSE)

GT, Improvement of Cement Staircase Construction Process for Developing Nations
Team Stairway to Heaven – K. Mason Brantley, John W. Golden, Paige Orangio, Tyler Rice, Tim Widing

Gulfstream Aerospace, Moisture Barrier Technology for Wood and Wood Finishes
Team MWA (Materials With Attitude) - Mackenzie Bolton, Ashley Hall, Patrick McGannon, Joseph Riordan, Kevin Smith, Bryan Vakiner

Hang on Holder LLC, Materials and Design Challenge
Gold Team – Francine Ejizu, Aaron Jordan, William Kennedy, Robert Rife, Jadzia Rivera

Printpack, Loading of Microcellulose in Polyethylene Based Composites for use in Flexible Sustainable Packaging
Team PolyPros - Jon Baldwin, Aijie Han, Amanda Luce, Graham Mellen, Kirsi Naidoo

Quantum Radiology, Bone Biopsy Tool
Team SkelExtract - Ransomed Adebayo (ME), Samantha Martin (BME), Shahnaz Kasam (ME), Marco Scaglia (MSE), Samuel Shackleford (MSE), Andrew Short (MSE)

Saint-Gobain, Design of a Quantitative Methodology for Assessing the Shear Stability of PTFE Dispersions
Team Fibrillation – Ashley Counsellor, David Kakalios, Wai Hong Lam, Kevin Low, Juan Irurita

Technetics Group Columbia, Design and Development of a Friction Test Bench
Team The Wreckening - Sean Bradley, Natalie Darby, Zachary Robbins, Hunter Smith, Noah Winter

Under Armour, Novel Properties of Acrylic
Team Group Squad - Rebecca Cohen, Nicole Kennard, Kelsey Novak, Andrew Sisung, Lindsey Thomson

Under Armour, Thermomechanical Failure of Hard Court Uniforms
Team Designers - Michael Davidson, Ryan Dwyer, Shawn Gregory, Christopher Lo, Keshav Swarup

Universal Fiberglass, Piping Selection Spreadsheet
Team Fiberglass Group – Randy Cheng, Jinho Hah, Benjamin Hatanpaad, Dohee Kim, Dudley Shannon

Need low cost skunkworks material design?
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Contact Mary Lynn Realff at 404.894.2496, marylynn.realff@mse.gatech.edu
or
Blair Brettmann at 404.894.2535, blair.brettmann@mse.gatech.edu
The Georgia Tech Polymer Network (GTPN) was created in 2012 to enhance the visibility and cooperation in Polymer Science and Engineering across the Georgia Tech campus. Many of our schools have faculty with strong polymer research and education efforts underway, with the School of Materials Science and Engineering leading the effort. GTPN's role is to “network” our faculty in the polymer science and engineering sub-discipline to make us stronger than the sum of our parts. The GTPN coordinates the efforts of our faculty to foster collaborative interactions, elevate our visibility through various forms of advertising and seminar programs, participate in faculty and student recruiting, and generate an atmosphere to initiate new cooperative research and teaching interactions.

With over 30 GT faculty members participating in the GTPN, creative teams are being established to compete for externally and internally funded programs of scale in polymer science and engineering. GTPN faculty are involved with a broad range of research topics such as developing new materials for a variety of applications including: nanoporous membranes for separations, electrode materials for batteries and supercapacitors, polymer-modified nanoparticles for drug and active molecule release, and electroactive conjugated polymers for displays and solar cells.

Over the last three years, the GTPN has sponsored over 40 academic, government, and industrial visitors to campus to get to know our research, ongoing projects, and facilities. These visits have been an especially important undertaking early in the life of the GTPN. Further, the GTPN is working to coordinate the numerous polymer science and engineering courses offered in the various schools across campus. By collecting these courses under one umbrella, students can more effectively determine the best set of courses for their own program. Our active Student Polymer Network participates in many activities, including welcoming new faculty to campus, presenting to the public at the Atlanta Science Festival, visiting nearby companies, participating in the outreach program, “Step into STEM,” which presents demonstrations to elementary and middle school children, and attending the National Graduate Research Polymer Conference in Akron, Ohio. John Reynolds, Director of GTPN, believes the impact on graduate students and researchers is an important component of the organization. “They’re not just increasing their knowledge of chemistry, physics, and materials science; they are growing professionally by participating in meetings and seminars, hosting visiting scientists, and learning how to professionally interact with others. Additionally, they develop contacts with companies which can lead to career opportunities.”

Student Polymer Network members Paul Balding, ChBE, Alyssa Blake, ChBE, Michel de Keersmaeker, ChBE, and Gus Lang, MSE, use household ingredients to make silly putty at the 2017 Atlanta Science Festival.
Seung Soon Jang

Computational Materials Science towards Designing Better Materials in Energy and BioTechnologies

Multiscale Modeling Paradigm

Computational materials science investigates fundamental mechanisms influencing a variety of properties of materials by using modeling and simulation to show the structure-property relationship, which then becomes an essential part of designing new materials with the most desirable properties.

In the context of a multiscale modeling paradigm (Figure 1), we primarily use three computational methods to determine the best structure-property relationship. First, we use an atomistic modeling approach because it is a tool with the highest resolution. In atomistic modeling, quantum mechanical methods, such as ab initio and density functional theory, are employed for a system consisting of ~10^2 atoms to study electronic structures and properties including binding energy, polarizability, ionization potential, and electron affinity. Next, molecular dynamics simulation, with the second highest resolution, is used to describe a materials system consisting of up to ~10^6 atoms. Using statistical mechanics, thermodynamic properties can be calculated from the equilibrium state, while time-resolved structural evolution and transport properties can be monitored through non-equilibrium process. The third computational method used is a coarse-grained mesoscale modeling method, which has the least resolution, to study the structures of up to ~10^{-6} m, in order to characterize morphological properties developed from phase formation. This third computational method can be combined with a finite element method for further analyses such as mechanical properties under certain applied stress condition, or electromagnetic response in an applied electromagnetic field.

By developing a multiscale modeling paradigm that consists of various methods with their unique temporal and spatial resolutions, we can understand the fundamentals of complicated material behaviors whose mechanisms are not restricted to just one of these three scales. Our multiscale modeling paradigm allows us to effectively investigate materials for energy and biotechnology.

Energy Materials

There is currently a great need to continue to improve sustainable and renewable energy technologies such as the Li-ion battery, which stores electrochemical energy in the cell and converts it back to electricity. For the Li-ion battery, we have investigated a molecular design of organic materials for electrodes (Figure 2). Using systematic DFT calculations of various organic materials including quinone derivatives, we found that the redox potential of the electrode can be tuned by designing molecular structure to adjust electron affinity. Through our studies, we have shown the effects of aromaticity and chemical functional groups on the redox
potential, concluding that the electron-withdrawing groups improve the redox potential (Journal of the American Chemical Society (2016), Energy and Environmental Science (2017)).

Another futuristic energy technology is to develop an energy efficient system for chemical reactions. By designing multiblock copolymers consisting of hydrophilic and hydrophobic chemical structures, molecular self-assembly such as micelle structure can be accomplished in solvent systems, which can then be used as a nano-reactor of ~10² nanometer size. The reactants can be thermodynamically driven into the nano-reactor and products are then pushed out via concentration gradient (Figure 3). Benefits of such nano-reactors include: 1) enhanced kinetics due to high catalyst concentration in the nano-reactor; 2) recyclability of resources such as catalysts and solvents; 3) and the capability for various cascade chemical reaction systems. In collaboration with experimental groups, we have been developing a multiscale modeling protocol ranging from quantum-mechanics to mesoscale simulations to develop this energy-saving chemical reaction technology (Physical Chemistry Chemical Physics (2015), Physical Chemistry Chemical Physics (2016)).

Bio Materials
Computational materials science can help reveal structures of materials and processes in bio-systems. For instance, in our research on dental materials, the bio-mineralization process was investigated using full-atomistic and coarse-grained molecular dynamics simulation methods (Figure 4). For this study, a collagen fibril model was developed via full-atomistic modeling. The overlap region of the collagen fibril has a densely packed collagen triplex structure, while the gap region has a water-filled void. We discovered that the collagen molecules in the gap region can undergo structural reorganization with the intrusion of an external solvent phase (Acta Biomaterialia (2016)). We also found that an external polymer electrolyte can facilitate the intrafibrillar collagen mineralization by transporting calcium phosphate through the Gibbs-Donnan mechanism (Nature Materials (2017)). Through this modeling-experiment collaborative research, the fundamentals of bio-mineralization mechanism were understood.

Seung Soon Jang is an associate professor in the School of Materials Science and Engineering at the Georgia Institute of Technology. Prior to joining Georgia Tech in 2007, Jang worked at Samsung Electronics and at the Materials and Process Simulation Center (MSC) at CalTech as Director of Supramolecular Technology. His research interests include computations and theories to characterize and design nanoscale systems based on molecular architecture-property relationships.

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Relating Microstructure to Failure Initiation in Extreme Environments

Our everyday interaction with failure in materials tends towards the large-scale and often catastrophic, such as a car axle breaking or, on a much larger scale, the collapse of a bridge. The origin of these failures, however, is at the nano to microscale, resulting from the accumulation of billions of atomic-scale defects and their interactions with a material’s microstructure.

The primary objective of the Kacher Lab is to discover the relationship between microstructure and failure initiation in a range of metallic systems with the goal of developing safer, more reliable alloys. To better understand the mechanisms driving damage accumulation and failure initiation, the lab develops and applies novel in situ electron microscopy techniques such as liquid cell corrosion and mechanical deformation that mimic real-world environments. Data collection rates associated with these electron microscopy experiments have dramatically increased over the last decade with the advent of advanced electron detectors and improvements in computational processing power to the point where terabytes of data can be collected over the course of a single experiment. These advances in data collection efficiency have increased the role of data analytics in electron microscopy characterization and have brought statistical relevance to the results.

The lab explores a wide range of material systems and environments, including fatigue and high strain rate deformation of additively manufactured steel and nickel alloys, ductile failure of steel and aluminum alloys, and corrosion processes in duplex steels and aluminum alloys. Two important areas currently investigated are the microstructural origin of ductile failure in heat-treatable aluminum alloys and the dependence of local corrosion susceptibility on microstructure in work-hardened aluminum alloys.

Heat treatable aluminum alloys such as Al 6061 are seeing increased use as lightweight alternatives to steels as structural components. A recent example of this is the extensive use of Al 6061 in the Ford F150. The microstructure of these aluminum alloys is composed of a complex array of precipitates, used to strengthen the material, dispersoids for microstructure control, and intermetallic constituent particles from impurity elements. To understand how these different components of the microstructure contribute to failure initiation, the Kacher Lab combines in situ scanning electron microscopy (SEM) deformation with electron backscatter diffraction (EBSD)-based analysis. EBSD relies on rapidly collecting diffraction patterns from a defined region on the surface of a material to map out the local crystal orientation and dislocation distribution. These deformation maps can then be compared to local characteristics of the microstructure, such as the distribution of precipitates or the average grain size, using correlation functions to better understand the role...
they play in failure initiation. Figure 1 demonstrates the effect of intermetallic particles on localized dislocation accumulation. In order to directly resolve the local dislocation structure, thin lamella of material are machined from areas of interest using a focused beam of gallium ions. These lamella can then be characterized via (TEM), facilitating the direct resolution of dislocation interactions.

Aluminum alloys are also increasingly used in naval applications where their high strength-to-weight ratio leads to lower fuel consumption and higher attainable speeds. However, the constant exposure to aggressive salt water environments has been observed to contribute to corrosion-related material failure. Corrosion attack of the aluminum alloys occurs primarily through a pitting mechanism where the passivation layer locally breaks down at a susceptible point on the material surface, resulting in the creation of a corrosion pit on the material surface.

The Kacher Lab employs a data-science based approach to correlate pit initiation sites with microstructure by comparing high resolution EBSD scans collected before exposure and then to a corrosive environment followed by the distribution of corrosion pits after corrosion has taken place. In addition to the EBSD-based experiments, corrosion processes can be characterized directly at the nanoscale using in situ TEM liquid cell experiments.

In these tests, a thin layer of aluminum is isolated between electron transparent Si₃N₄ chips and corrosive liquid is flowed over the sample. Figure 2 shows an example of a corrosion pit initiating and expanding through the material in a model iron system. These tests provide information on how corrosion fronts propagate through a material, in addition to insight into the nanoscale processes dictating corrosion susceptibility.

Josh Kacher is an assistant professor of Materials Science and Engineering at the Georgia Institute of Technology. His primary research interests are in relating the performance of materials in extreme environments to their microstructure and processing history. This includes understanding how environmental factors such as elevated temperature or corrosive elements affect the mechanical properties and failure modes of materials. These phenomena are investigated primarily using novel in situ transmission and scanning electron microscopy techniques.

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Polymeric materials are used ubiquitously to meet societal needs. They appear in familiar areas such as healthcare, transportation, food and beverage packaging, and apparel, as well as emerging areas such as flexible electronics and renewable energy. Among other attributes, the facile processing and structural diversity of polymers have led to their pervasive presence in modern society. The Shofner research group investigates these aspects of polymer engineering with a goal of discovering effective materials design strategies for polymers and filled polymer systems. In recent work, her group has applied this strategy to diverse systems such as cellulose nanocrystal composites, auxetic fiber networks, and tensegrity-inspired polymer composites.

Cellulose nanocrystals are a nanofiber form of cellulose that has become widely available to researchers from domestic and international suppliers. This increased supply has been the impetus for increased research activity with these materials by the filled polymer and composite communities. These nanofibers consist almost entirely of ordered cellulose macromolecules and are derived from bio-synthesized cellulose structures in plants, organisms, and some animals. They are predicted to have high specific mechanical properties, making them attractive choices as reinforcements for polymers. Shofner's research group has explored how to use cellulose nanocrystals in composites as a performance additive and as the majority component similar to conventional fiber composites. Much of this work has been performed in collaboration with J. Carson Meredith in the School of Chemical and Biomolecular Engineering and scientists at the US Forest Service's Forest Products Laboratory. The results have shown that cellulose nanocrystals may be used to improve the thermomechanical performance of polymer coatings, to change the curing kinetics of thermosetting polymers, to nucleate polymer crystallization, and to increase the work of fracture of polymers. Current work is focused on the use of cellulose nanocrystals in packaging materials to enable higher performance and more sustainable materials options. Figure 1 shows a polarized optical microscopy image of one such composite, a cellulose nanocrystal/poly(ethylene-co-vinyl alcohol) composite with an anisotropic composite structure.

The Shofner research group has also pursued the production of auxetic fiber structures. Auxetic materials/structures have a counterintuitive response to deformation. Specifically, these materials and structures exhibit a negative Poisson’s ratio, meaning that they expand when stretched or shrink when compressed. Materials and structures with a negative Poisson’s ratio are finding applications in damping, shock absorption, and composites with mechanically interlocking interfaces. In collaborative research with AnselM Griffin in the School of Materials Science and Engineering, the group has investigated how to use the structure of needle-punched nonwoven fabrics made from polymer fibers to achieve an auxetic response in tension. By subjecting the as-produced fabrics to heated compression, a Poisson’s ratio of approximately -12 has been attained, producing a dramatic and
visible auxetic response when the fabric is deformed. The mechanism for auxeticity is related to the highly entangled fiber structure and the recovery of tilted and/or buckled needle-punched pillars upon the application of tensile deformation. Figure 2 shows the structures for an as-received and heat compressed fabric, i.e. the densification of the structure and change in the needle-punched pillars caused by the heated compression step. Overall, this process of producing an auxetic structure from fiber networks is general and can be applied to other needle-punched nonwoven fabrics as well as other types of nonwoven fabrics and structures.

Tensegrity is a contraction of the phrase “tension integrity” and describes a system that contains discrete compressed elements connected by a tensioned web. It has been used as a design concept in architecture and art. Increasingly, the concept of tensegrity is being applied to examples in nature and biology such as mechanotransduction in cells. Beyond natural systems and materials, aerospace applications have sought to use tensegrity as the design concept for deployable structures, allowing the structure to be compactly packed for transport. The Shofner research group has used tensegrity principles as inspiration for the design of polymer nanocomposite microstructures in films with the motivation of improving mechanical properties of discontinuously reinforced nanocomposite materials. The concept of tensegrity is applied to nanocomposites by considering the nanoparticles as the compressed components and the surrounding matrix as the tensioned element. Drawing operations were used to apply prestress in the matrix and to arrange the compressed components in the polymer matrix simultaneously. Comparing the thermomechanical properties of the tensegrity-inspired polymer nanocomposite to those of the starting nanocomposite and a nanocomposite with uniaxially oriented nanoparticles, the results suggested that tensegrity-inspired approach produced improved mechanical performance at temperatures below the glass transition. Additionally, the results showed that this processing strategy was more effective with semicrystalline polymer matrices, suggesting that the topological constraints at the amorphous/crystalline interface in the matrix assisted in forming the tensioned web needed for tensegrity.

Meisha Shofner is an associate professor in the School of Materials Science and Engineering and an associate director of the Renewable Bioproducts Institute at the Georgia Institute of Technology. Her research focuses on the processing-structure-property relationships of filled polymers, with particular emphasis on bio-based materials and processing strategies that produce hierarchical structures. The research described here has been supported by the Renewable Bioproducts Institute at Georgia Tech, the US Forest Service, and the National Science Foundation under Grant No. CMMI-0800019.

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Alumni Advice

Words of Wisdom for the Next Generation

Morgana Trexler, M.S. MSE '05, Ph.D. MSE '08, Supervisor, Multifunctional Materials & Nanostructures Group at John Hopkins University Applied Physics Laboratory

It is important to have the ability to learn quickly and apply critical thinking to a broad range of topics. We work on a huge variety of materials and applications and need to be able to contribute even without specific background in any particular area. Also, effective communication of ideas and results is critical to creating vision, developing new projects and capabilities, and conveying importance of findings.

Matt Trexler, Ph.D. MSE '07, Director of Technology Validation, Under Armour, Inc.

Remember that well trained students are ultimately what universities are supposed to produce. These days, many professors are forced to concentrate on research funding or high impact papers, to spinning off start-ups. These things are important, but the students and the training of the next generation of engineers must always come first. Managing these pressures can be difficult but finding several good mentors can help a great deal.

Ryan Kincer, Ph.D. PTFE '11, Materials Engineer, Naval Surface Warfare Center, Dahlgren Division

Science is fun. That is a concept we all learn as young kids but we often lose that notion as an adult with the next deadline always looming. I think it’s important to always celebrate the positives and be encouraged by the failures knowing that you are learning either way.

Michelle Kincer, B.S. PTFE '06, Ph.D. PTFE '11, Materials Engineer, Naval Surface Warfare Center, Panama City Division

The most important key to innovation is diversity. Our group is made of varying disciplines and backgrounds. Each person is versatile and can fill multiple roles as the need arises. Concentrate and do well in your specialty, but be prepared and humbled to continue learning until long after retirement.
Travel with an Eye on Materials

Learning from everyday experiences has been a consistent theme that Regents’ Professor Tom Sanders has imparted over his entire teaching career. More recently, Sanders has been teaching MSE 2001, Introduction to Materials Science and Engineering, to study abroad students at Georgia Tech Lorraine (GTL).

Located in Metz, France, the GTL study abroad program offers undergraduates a unique opportunity to explore Europe and develop an understanding of its diverse geographies and people. The area in and around Metz offers a unique glance into the history and application of materials. Here are a few highlights of travel with an eye on materials that Sanders emphasizes to his students.

Taking two years, two months, and five days to build, the Eiffel Tower was constructed using iron from the Lorraine region. Built for the Exposition Universelle of 1889 and selected from over three hundred entries for its striking design and economy of structure, the Tower displays the French prowess in metal construction. Painting the Tower has protected the iron from oxidation and is the essential element in its conservation. The metal structure of the Tower weighs over 7,300 tons, and is built from 18,000 different parts with 2,500,000 rivets.

Le Mont-Saint-Michel is an island community in France where Normandy and Brittany merge. From 966 onwards, the Benedictine abbey on the island became a renowned center of learning, attracting some of the greatest minds and manuscript illuminators in Europe. Ramparts at the base as well as quicksand surrounding the island kept English forces out. Students are encouraged to explore the rheology of this sand water mixture, for unlike in the Tarzan movies, humans float in quicksand.

Water from the Dordogne and Garonne Rivers color the Gironde Estuary, on the western coast of France, making the river appear dirty. The water moves very quickly and stirs up the clay particles and sediments. Flocculation (the condition in which clays, polymers or other small charged particles become attached and form a fragile structure) creates a floc resulting in a dispersed clay slurry. Flocculation occurs after mechanical agitation ceases and the dispersed clay platelets spontaneously form flocs. This flocculation is possible because of attractions between negative-face charges and positive-edge charges as a result of a chemical reaction between the clay particles and in this case the salt water. Even though the Garonne is brown and appears dirty, students learn that this river is among the cleanest rivers in Europe.
Electron micrograph of a fuel cell composite electrode of molybdenum carbide and doped barium cerate after exposure to high temperature annealing, taken by graduate student Brian Doyle from the Meilin Liu group and enhanced with false color by undergraduate Lovelyn Wirian in The MILL.