Getting Smart About AI

Artificial intelligence is revolutionizing materials characterization and design.

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Greetings to our MSE alumni! As I write this letter, the Department of Materials Science and Engineering shares equal portions of opportunities for the future — resulting from those things we control — and significant challenges resulting from external factors we cannot control. On balance, the Department continues to thrive, as evidenced in the stories in this issue of MSE News.

As everyone is aware, the COVID-19 crisis has been an enormous challenge for the University. Team activities, interpersonal interactions, hands-on experimentation, and experiential learning are all essential elements of our education program that have had to change to operate safely. As one would expect of our faculty and staff, they are being creative and working hard to adapt so we are able to advance our research and education mission. While this has created an additional burden for our community, we carry on recognizing that we are fortunate to be doing this, while others are suffering because they have lost their health or their jobs during this crisis.

The best news we have had this summer is that Professor Elizabeth Dickey has accepted an appointment as the next Head of Materials Science and Engineering. Beth is a gifted professor with excellent administrative experience, including managing materials characterization facilities, directing a graduate education program, and serving as Associate Department Head at North Carolina State University. She is also an accomplished researcher and has been the principal investigator for the Center for Dielectrics and Piezoelectrics at NCSU. Beth’s focus on microscopy and interfaces integrates well with the Department’s research interests and infrastructure. More information about her will be provided in the next issue of MSE News.

In this issue, I draw your attention to the cover story on how artificial intelligence is revolutionizing materials science and engineering. This is a rapidly growing field in the College of Engineering, and the MSE Department is strongly engaged with both research and education in this area. This issue also contains many updates about students, faculty, alumni, and staff, including a story about how one of our students developed a medical device that can be used in the treatment of COVID-19 patients.

I hope you enjoy reading about the other activities and achievements of MSE faculty and students. Please let us know of any significant developments in your career and life that we can feature in future issues. As always, if you are in town and have the opportunity, you are always welcome to visit the Department. This year, the MS&T meeting is scheduled to be in Pittsburgh in October; assuming the meeting is held, I hope to see you there.

GREGORY S. ROHRER

A NOTE FROM THE DEPARTMENT HEAD
Gregory S. Rohrer
W.W. Mullins Professor
Artificial intelligence is revolutionizing materials characterization and design — and MSE’s Elizabeth Holm is at the forefront of this effort

With a dual Ph.D. in MSE and Scientific Computing, Professor Elizabeth Holm has always been a leader in leveraging the latest computational tools to understand and elucidate materials characterization. Today, her lab in the MSE Department at CMU is a global leader in applying artificial intelligence (AI) to automate and accelerate many characterization activities — as well as create new, customized materials.

“As computational advances have made AI much more accessible, it is changing our world," says Holm. “It’s exciting to apply these advanced capabilities to help solve pressing challenges in materials science and engineering.”

Working Smarter and Faster
As one example, Holm points to the significant benefits of AI for the microstructural characterization of materials. “Since the 1800s, scientists have analyzed the microstructure of materials manually, looking at constituents and physically measuring and counting them,” she notes.

“Today, AI can apply human-like judgement to the process of segmentation and completely automate this activity — quickly presenting the results to a scientist,” explains Holm. “We can make much faster and more meaningful strides in understanding how the constituent make-up affects material properties such as strength or fracture resistance.”

Greater-Than-Human Perception
Not only does AI speed up common tasks, but it adds a new layer of perception that can augment and sometimes surpass the human eye and brain.

For instance, Holm is applying computer vision and machine learning to detect toxic particulates that could be harmful if inhaled — and distinguish them from benign particulates. While associating toxicity with various particle types is currently a human task, AI-based perception systems can be “trained” to recognize the subtle characteristics of toxicity, via machine learning. That the AI system can achieve near-human performance with considerably higher throughput is a major advantage of this system. However, a more subtle benefit is augmenting human vision with a different, complementary machine perception.

“What exactly is AI seeing? In many cases, we don’t know,” Holm admits. “Two particulates might look identical to the human eye, but AI can recognize minute differences that are not part of how humans process an image. It’s an incredibly powerful perception capability that is changing the nature of microstructural science.”

A New Level of Materials Customization
Equally exciting is the potential for artificial intelligence to suggest entirely new, customized materials microstructures with targeted properties.

Generative adversarial neural networks can learn the characteristics of visual images well enough to produce convincing “fake” images. Working with large, three-dimensional microstructural data sets in CMU’s J. Earl and Mary Roberts Microstructural Characterization Facility, Holm has shown that this approach works in 3D as well. “We use AI to generate ‘fake’ 3D microstructures that are provably similar to the real ones in both structure and properties,” says Holm. “We use these synthetic microstructures to augment limited and expensive experimental data and perform statistical surveys of materials behavior.”

“Our ultimate goal is to start with a material property — such as fracture toughness — and use a generative network to predict a structure that meets a target for that property," Holm adds. “This is the perennially difficult inverse problem: designing a material structure to achieve custom performance.”
While the COVID-19 pandemic has closed MSE’s physical facilities, the sense of community remains strong

On March 16, in light of the growing COVID-19 pandemic, Carnegie Mellon moved to virtual instruction — and the Department of Materials Science and Engineering entered the age of working, teaching and learning remotely. The transition has not been without its challenges, but the MSE community has pulled together to remain connected throughout this global crisis. MSE News recently interviewed faculty, staff, and students to get a sense of how this experience has impacted them.

While Aharon Inspektor has a long history with MSE — including serving as an Adjunct Professor since 2015 — he assumed the role of Faculty Director for the Department's Masters Programs in October. Fortunately, he and the graduate team — Paige Houser, Senior Academic Advisor, and Jeanna Pekarcik, Graduate Admission Coordinator — were able to hold an on-campus, open-house event before the onset of COVID-19, where he presented the masters degree programs for 2020. This was followed by two international open-house events via the Zoom videoconferencing app and extensive Q&A email exchanges. As helpful as these are, Inspektor misses the face-to-face, one-on-one connections with students. “Starting from the moment the students get on campus until they will graduate, I want to be physically present for them as a coach and a cheerleader,” he explains. “From help choosing their classes to discussing their long-term career plans, my role is to ask tough questions and make them think about the impact of their decisions.” Inspektor has already formed close relationships with MSE students as an adjunct faculty member, and during his 24-year career as a Senior Scientist at Kennametal, where he conducted joint research projects with MSE. As a member of many academic-industry boards and journal editorial boards, co-author of over 40 papers, and owner of 20 patents, Inspektor brings an incredible wealth of insight and mentor expertise to his new role at MSE. “Whether students are looking toward a career in industry, or in academia, I want to help them make the right choices to realize those goals,” says Inspektor. “Hopefully, we can soon begin talking about these important topics in person. But for now we are using the best available technologies to connect remotely, no matter where in the world the students are. I look forward to the day when they are physically here on campus.”

The concept of remote instruction might be new to many members of the MSE community. But, for Graduate Admissions Coordinator Jeanna Pekarcik, it’s second nature. In fact, in December Pekarcik won the College of Engineering’s Burritt Education Award for balancing her work at CMU with her pursuit of an online bachelors degree in Organizational Leadership at Point Park University. Since Fall 2018, she has taken two classes each semester at Point Park, while managing the admissions process for all MSE masters and doctoral students. In addition, Pekarcik supports seven MSE faculty members. While working online is a relative breeze for Pekarcik, the stay-at-home order means she is now also managing remote schooling for her nine-year-old daughter Sadie. “There’s nothing cuter than seeing an entire class of third-graders congregating on Zoom for their math class,” says Pekarcik with a laugh. “I love my job at MSE, I love my classes at Point Park, and I love being

< Jeanna Pekarcik receives the Burritt Education Award from CIT Dean William Sanders
a mom — but the pandemic means I am doing all three things simultaneously. The Burritt Award recognized my capabilities for work-life balance, and I am certainly earning it right now.” Pekarcik is grateful for the support she has received from her coworkers in the MSE Department for the past 15 years, including during the current crisis. This hard-working MSE team member hopes to apply the leadership and management skills she is learning at Point Park to take on even greater responsibilities in the future.

MSE doctoral student Zihao Ding actually had an early glimpse of the impact of COVID-19 based on reports from his family in China, where his mother works as a nurse. “Back in January, my family warned me that I would need personal protective equipment and face masks,” he recalls. “The Chinese embassy sent me a health care kit in advance. This situation, while new to most Americans, is something my family has experienced before.” Since Ding’s doctoral research focuses on the computational simulation of material layers to assess and improve their structural properties, he is able to complete his work on a laptop while working remotely. He admits that living alone during a pandemic is challenging, but credits his advisor, Professor Marc De Graef, and fellow MSE doctoral students for helping him stay connected to the outside world. “We meet regularly one-on-one, as well as in research groups,” Ding notes. “Everyone has made an effort to keep in touch, and that means a lot.” He and De Graef are continuing to collaborate on research. With Postdoctoral Research Associate Elena Pascal, they are co-authors on a paper titled “Indexing of Electron Backscatter Diffraction Patterns Using a Convolutional Neural Network” that they hope to publish soon. On a personal note, Ding is thankful for the resilience and dedication of those working at the front lines, both in Pittsburgh and around the world. “I really want to express my gratitude to all the medical staff, police, mail carriers, and others who are staying at their positions during the pandemic,” he says.

Chloe Lenker, a sophomore with a dual major in MSE and Biomedical Engineering, is remaining on campus during the stay-at-home order. “I’m a resident assistant in the CMU dorms, and I volunteered to stay because so many of our international students are unable to return home at this time,” Lenker explains. “The only huge challenge was moving very quickly to a new dorm, where everyone can have a private room and bathroom for health reasons. It was tough to do on short notice, but we are settled in now.” Lenker has been taking six remote classes, and she appreciates the support and accommodation of MSE faculty. “When I was asked to move, it was hard for me to complete some assignments on time,” she notes. “Other students have their own challenges, like having classes in the middle of the night in their time zones. But all the professors have been very understanding as we adapt to the new normal.” She notes that, while it is difficult to replace hands-on opportunities in the lab, the faculty are conducting live demonstrations that have been helpful. Lenker has had to make other sacrifices, including the cancellation of a fully funded research-abroad trip to Israel as part of the International Summer Undergraduate Research Fellowship (ISURF). She was planning to develop nanoscale drug delivery systems for the nervous system at The Technion — Israel Institute of Technology. She hopes to re-apply for funding and complete this trip in 2021.
CMU and AFRL Form Center of Excellence

Carnegie Mellon has partnered with the US Air Force Research Laboratory (AFRL) to create a five-year Center of Excellence initiative focused on data-driven materials research. By leveraging $7.5 million in funding — along with each partner's expertise in data science, computer vision, artificial intelligence (AI), and materials characterization — the partners will advance the state of materials research. The Center’s goal is to develop next-generation aerospace materials, establish a pipeline of research talent with both AI and materials science expertise, and advance the materials science field by integrating AI into materials research and design.

Called “Data-Driven Discovery of Optimized Multifunctional Material Systems (D^3OM^2S),” the Center is supported by an award from the Air Force Office of Scientific Research (AFOSR) and the AFRL Materials and Manufacturing Directorate.

At Carnegie Mellon, the Center is led by MSE’s Professor Elizabeth Holm and includes interdisciplinary faculty experts from Mechanical Engineering, Electrical and Computer Engineering, the Robotics Institute, and Computer Science. Other MSE faculty investigators include Professors Michael Bockstaller, Marc De Graef, Gregory Rohrer, and Anthony Rollett. Lead personnel from CMU and AFRL gathered in Pittsburgh in December to kick off the partnership.

According to Holm, Carnegie Mellon was awarded this prestigious partnership because of its deep expertise in materials characterization, computational science, and machine learning. The Center will focus on four major research thrust areas: characterization and prediction of rare events in materials, multimodal data fusion, adaptive experimental design, and adaptive materials design in complex environments.

“We had to be a leader in this space to be competitive for this award in the first place,” says Holm, “but this is the type of transformative support that will establish CMU at the forefront of the materials science – data science interface for years to come.”

Rollett Wins $2.4 Million DOE Research Grant

Professor Tony Rollett and his MSE research team have received a $2.4 million grant from the US Department of Energy (DOE) Advanced Research Projects Agency – Energy (ARPA-E) to support their research of high-temperature materials and heat exchangers. The grant will help Rollett’s group explore new methods for additive manufacturing — commonly known as 3D printing — that will help accommodate new, more efficient heat-exchanger geometries. The DOE funding will support Rollett’s research for three years.

Heat exchangers are devices that transfer heat from one fluid to another, without the two fluids coming into contact with one another. They are commonly used in the engines of cars, ships, and planes, and in heating and cooling systems, including air conditioners and refrigerators. The overall ARPA-E initiative supports the creation of critical heat exchangers for use in electricity generation, nuclear reactors, transportation, and other applications where they will experience high temperatures and other harsh operating conditions.

“The particular challenge is that we have to be able to print these heat exchangers, because the only way to make them efficient enough, and in fact modular enough, is through 3D printing,” notes Rollett. “3D printing allows us to have much more variation in the geometry, much more arbitrary geometry.”

As part of the project, Rollett will also explore different alloys and materials that haven’t been used before. “This is a wonderful opportunity to demonstrate how 3D printing helps in an advanced application, and it also gives us an opportunity to, if not develop brand new alloys, at least bring new and different alloy compositions into 3D printing,” adds Rollett.
A Clearer Picture of Crystals and Structural Defects

Professor David Laughlin and Caroline Gorham, a Postdoctoral Research Associate in MSE, have published a paper that considers a novel framework to more effectively understand crystallization, the process through which a liquid or gas is transformed to a solid. The team is especially interested in studying crystalline solids that contain permanent structural defects by applying concepts of topology — a field in mathematical physics concerned with the properties of materials that remain unaffected by deformations such as stretching, bending, and twisting, but not cutting or gluing.

The paper, titled “Crystallization in Three Dimensions: Defect-Driven Topological Ordering and the Role of Geometrical Frustration,” appeared in the April 19 edition of *APS Physical Review B*. This paper is the most recent in a series of publications in which Laughlin and Gorham work to elucidate the largely unexamined process of imperfect crystallization.

Bettinger Elected to AIMBE College of Fellows

Professor Christopher Bettinger has been elected to the American Institute for Medical and Biological Engineering (AIMBE) College of Fellows, Class of 2020. Bettinger holds a dual appointment in MSE and Biomedical Engineering. He directs the Laboratory for Biomaterials-based Microsystems and Electronics at CMU, which designs materials and interfaces to integrate medical devices with the human body. Representative examples of Bettinger’s work include the design and synthesis of novel materials and devices to improve the reliability of neural interfaces; the use of flexible electronics for non-conventional neural interfaces; and adhesives for use in soft electronics and surgical materials.

Election to the AIMBE College of Fellows is among the highest professional distinctions accorded to a medical and biological engineer. The College of Fellows is composed of the top two percent of medical and biological engineers. AIMBE Fellows have made outstanding contributions to “engineering and medicine research, practice, or education” and to “the pioneering of new and developing fields of technology, making major advancements in traditional fields of medical and biological engineering, or developing/implementing innovative approaches to bioengineering education.”

De Graef Chosen for TMS Fellow Award

Professor Marc De Graef has been named a 2020 Fellow of The Minerals, Metals & Materials Society (TMS). According to a TMS statement, De Graef was recognized “for pioneering scientific and educational contributions to the quantitative characterization of magnetic materials and 3-D material microstructures.” De Graef’s current research focus is on the development of experimental and modeling techniques for the quantitative study of magnetic domain configurations in a variety of materials, including ferromagnetic shape memory alloys, magnetic thin films, and patterned structures.

The Class of Fellow is TMS’s highest honor. To be inducted, a candidate must be recognized as a leading authority and contributor to the practice of metallurgy, materials science, and technology. This includes scholarship, such as the publication of articles or books; the granting of patents; direction of important research or engineering work; and responsibility through management for nationally known improvements and developments in the field. A strong consideration is also given for outstanding service to the Society.
Marom Explores New Materials for Solar Cells

Professor Noa Marom is the Principal Investigator on a cross-institutional, cross-disciplinary effort to identify new materials that make photovoltaic solar cells more efficient. The team’s investigative methods rely on machine learning, which makes their work computationally intensive and numerically large.

To help manage this mathematical workload, the US Department of Energy’s Argonne National Laboratory has granted the team early access to Aurora, an emerging exascale computer. The project led by Marom is one of just 15 efforts selected to access Aurora by the Argonne Leadership Computing Facility (ALCF) through its Early Science Program (ESP). These elite projects support the ALCF’s efforts to create an environment that enables data science and machine learning approaches alongside traditional simulation-based research.

Says Marom, “The goal of our research is to find new materials that make photovoltaic solar cells more efficient via their unique properties. However, these properties are very rare and difficult to identify. We are trying to accelerate the process of material discovery through computer simulation on high-performance computers, using sophisticated quantum-mechanical simulation software and machine learning.”

“We are excited that our project has been accepted as one of the projects that will run on the future Aurora supercomputer as part of the Argonne ESP program,” she adds, “Our multi-institution team is currently modifying algorithms and workflows so they will be able to run on Aurora.”

Co-Principal Investigators on the team include Jack Deslippe from Lawrence Berkeley National Laboratory, Luca Ghiringhelli of the Fritz Haber Institute of the Max Planck Society, and Barnabás Póczos, Associate Professor of Machine Learning at CMU.

Studying Steel Inclusions via Computer Vision

Professor Bryan Webler and Professor Elizabeth Holm are leveraging computer vision and machine learning techniques to study steel inclusions, hoping to make the characterization of these microscopic particles faster and less expensive. They shared their initial findings at the 2019 conference of the Association for Iron & Steel Technology.

Inclusions are microscopic particles within steel that have a big impact on its properties and can affect its ultimate performance. Steelmakers need to analyze them for quality control — and Webler and Holm aim to improve this process by applying computer vision and machine learning. Using inputs from scanning electron microscopy (SEM), machine learning engines can automate the process of gathering information on inclusions’ size, shape, location, and composition. This analysis, which would take a human several hours, is significantly accelerated.

The team’s early results are encouraging. In assessing SEM images, their computer vision techniques determined with 98% accuracy whether a feature was an inclusion or not. Even more impressive, differentiating each feature as an inclusion took their proprietary algorithm just 70 milliseconds.
MSE alum Michael Kurniawan works at the forefront of application-oriented semiconductor designs

As the world grows more digital, optimizing the performance of semiconductor chips is a critical challenge. As a Principal Design Engineer at GlobalFoundries, Michael Kurniawan (M.S. and Ph.D., 2015) is exploring improvements in chip designs that will power a new generation of intelligent devices and deliver significant benefits.

“It’s incredibly rewarding to be part of a multidisciplinary team leveraging advanced technologies to produce faster, smaller, and more efficient microchips for custom applications,” says Kurniawan. This MSE alum has taken a leadership role in defining and documenting technology specifications for GlobalFoundries’ products, bringing together data from multiple hardware, software, intellectual property, and business unit teams.

“Solving this kind of challenge requires both a team approach and a very detailed level of analysis,” Kurniawan points out. “For example, by performing mathematical modeling and statistical analysis in collaboration with hardware and software teams, we’re exploring improvements not only in ultimate chip performance, but the manufacturing processes used to produce chips. Through our analysis done in the last few years, we have significantly improved the quality of our Design Manuals and reduced some analytic work by more than 500 hours annually through automation.”

A NATURAL PROBLEM SOLVER

Kurniawan’s work at GlobalFoundries is an extension of the problem-solving approach he first applied as a Project Officer in the Physics Department at Nanyang Technological University in Singapore, after receiving his B.S. there in 2009. He led research aimed at understanding the physical mechanisms responsible for the power conversion efficiency of solar cells.

In 2012, he joined MSE as a graduate student in the lab of Professor Michael McHenry. According to Kurniawan, the intellectual freedom provided by McHenry was key in taking his problem-solving skills to the next level.

“My goal was to explore new soft magnetic materials for power, electric motor, and sensing applications, which would duplicate the performance of expensive boron-based soft magnets, at a much lower cost,” explains Kurniawan. “Professor McHenry took a very hands-off approach in advising my research. He would give me small bits of information — almost like leaving me a trail of breadcrumbs — and then let me find my own path.”

“My experience at MSE taught me to be independent and proactive,” he continues. “I realized that a key part of getting the right answers is asking the right questions. I had to look at the big picture before I could solve the smallest problems.”

Kurniawan notes that MSE proved the perfect training ground for his work at GlobalFoundries. “Today, I am attempting to solve a huge problem which will have an enormous impact on the world,” he says. “But that change needs to begin at the micro scale.”

PREPARING FOR A NEW CHAPTER

Kurniawan’s professional success has been matched by an equal measure of personal happiness. Prior to coming to CMU, he met a young woman named Rebekah in Singapore. During his almost three-and-a-half years in Pittsburgh, the two maintained a long-distance relationship. “We Skyped almost every day and saw each other virtually whenever possible,” he recalls. “It was difficult, but we knew we would be physically together one day.”

When Kurniawan graduated in 2015, the couple reunited in Pittsburgh to announce their engagement. Then they moved together to upstate New York when he joined GlobalFoundries. They are expecting their first child this summer.

“I will always remember my time in Pittsburgh fondly,” notes Kurniawan. “I’m grateful to the MSE Department for my education, which I am still applying every day.”
Dilara Ozdoganlar, a sophomore majoring in MSE and Biomedical Engineering, has been using her free time during the campus shutdown to support medical teams treating COVID-19 patients. She has been collaborating with a friend and fellow BME student at John Hopkins, Aydin Turkay, to design and make acrylic boxes that allow medical personnel to intubate patients without risking personal exposure.

“We first learned about this need from Aydin’s father, Dr. Atac Turkay, who is a physician at Heritage Valley Health System,” Ozdoganlar explains. “Intubating critically ill COVID-19 patients is a necessary procedure that helps them breathe. But it exposes health care workers to a large concentration of respiratory droplets and significantly increases their own exposure. A doctor in Taiwan pioneered the idea of building a protective structure to shield medical staff during intubation, and we were inspired by that idea.”

Working with Dr. Matthew Woodske, an intensive-care physician at Heritage Valley, Ozdoganlar and Aydin Turkay drew the specifications for a clear acrylic box that allows health care workers to visualize the patient. There are armholes on the front, through which a physician can conduct the intubation procedure. A second set of holes on the box's side allows a nurse to assist.

Two prototype boxes have already been made by Aqua-World, a local aquarium manufacturer, and are already at use in an intensive care unit at Heritage Valley. Based on feedback from doctors there, Ozdoganlar and Turkay are updating their design — and hope to produce more boxes that can be deployed at the frontlines of the COVID-19 pandemic.

A pre-med student, Ozdoganlar has found that her desire to become a physician is only strengthened by the current global health crisis. “I’m happy that I can contribute in some way during this pandemic, but I only wish I could do more,” she says. “It’s amazing to witness the efforts of the world’s health care workers today. I look forward to the day when I can be an active part of their heroic efforts.”

**NEWS BRIEFS**

**Aparna Jaggi** has been named a James R. Schwartz Entrepreneurial Fellow. An MSE-ETIM dual degree student, Jaggi graduated in May with two degrees: a masters in Materials Science & Engineering and a masters in Engineering & Technology Innovation Management. Awarded by the Swartz Center for Entrepreneurship at Carnegie Mellon, this fellowship fast-tracks the careers of CMU graduate students who are passionate about entrepreneurship in the technology arena. The highly selective program develops each Fellow’s entrepreneurial potential and leadership skills through hands-on experiences, networking, mentoring, and courses in entrepreneurship. Jaggi’s research interests lie in the field of energy storage devices, and she is passionate about bringing innovative ideas to the market. This fall, Jaggi will be joining Ernst & Young (EY) Foundry, the corporate venturing unit focused on creating transformational growth for EY and their clients by investing in and launching new digital businesses.

**Xining Gao**, a dual major in MSE and Biomedical Engineering who graduated in May, is a 2020 recipient of funding through the National Science Foundation (NSF) Graduate Research Fellowship Program (GRFP). The oldest graduate fellowship of its kind, the GRFP recognizes outstanding graduate students conducting research in the fields of science, technology, engineering, and mathematics. Each GRFP Fellow receives a three-year annual stipend of $34,000, along with a $12,000 cost-of-education allowance. Awards can be used for international research or at any accredited US institution of graduate education.
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Carnegie Mellon University publishes an annual campus security report describing the University's security, alcohol and drug, and sexual assault policies, and containing statistics about the number and type of crimes committed on the campus during the preceding three years. You can obtain a copy by contacting the Carnegie Mellon Police Department at 412-268-2323. The security report is also available online.


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