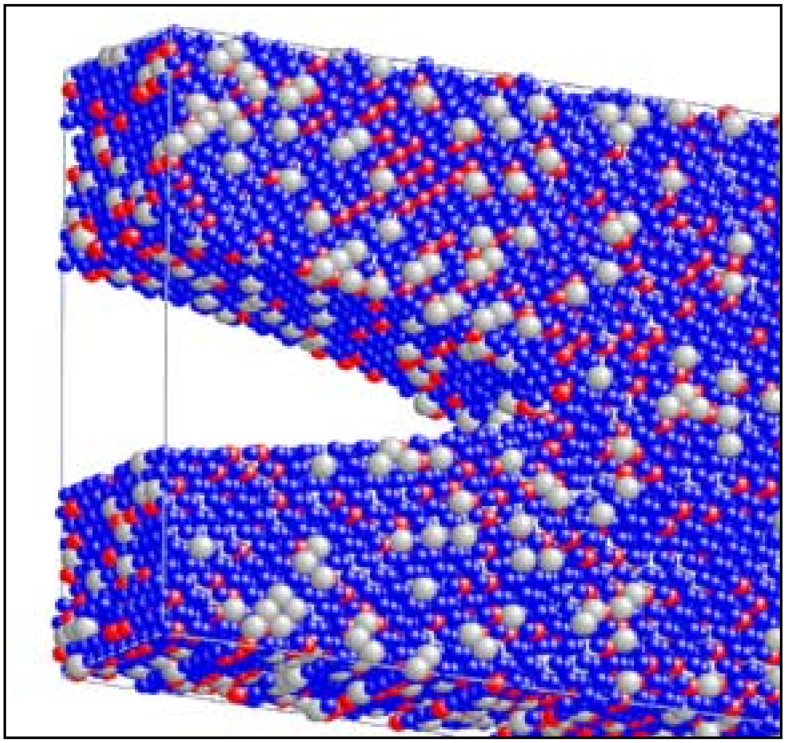
Exploring Materials

at Virginia Tech

Fall 2001, Volume 6, Number 2

News from the Department of Materials Science and Engineering
Virginia Polytechnic Institute and State University



Courtesy Diana Farkas

Three-dimensional atomistic simulation showing a crack in an Nb(blue)-Ti(gray)-Al(red) alloy.

In this issue...

Atomistic Simulation: A Useful Tool in Fracture Studies

LeeAnn Ellis

A particularly interesting problem in the study of fracture mechanics deals with understanding the mechanisms of energy dissipation that occur as a crack advances. In order to understand what is really happening, it's necessary to study the crack at the atomistic level. An experimental study might indicate, for example, that a crack tip is sharp and therefore may be the result of a brittle fracture. Atomistic simulation can be essential in understanding the precise activity at a crack tip as a fracture is advancing and can reveal that a crack thought to be sharp is not sharp at all.

Using atomistic simulation studies, researchers can observe energy-dissipation mechanisms in the crack-tip region and can obtain atomic configurations of that region under a variety of loading conditions. Professor Diana Farkas has been able to show that simulation studies and observations are useful in establishing correlations and trends, which can then be used to guide experimental development. For example, Dr. Farkas has used atomistic simulation to study fracture in intermetallics. In this case, studies have shown that, as a tendency

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Virginia Tech

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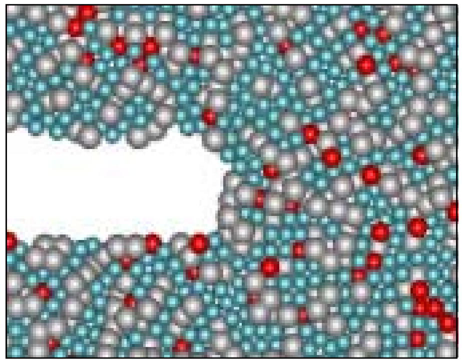
Research Corner

Simulation Continued

for ordering is decreased in an intermetallic, the resulting trend is an increase in fracture toughness. Such a trend can then act as a guide for the experimental development of intermetallic alloys, which are particularly useful in the aerospace and aeronautic industries for structural applications.

Professor Farkas has concentrated her research efforts on the structure of defects in alloys and the relationship of these structural characteristics to materials behavior. She focuses on modeling techniques for the study of alloy properties and has performed modeling work in various metallic alloys for ion-implantation processes and atomistic structure of defects as well as transport properties. Recently, she has worked on the creation of three-dimensional, virtual-reality visualization of structure defects and fracture behavior at Virginia Tech. Examples of both two- and three-dimensional simulations can be viewed at:



Courtesy Diana Farkas

Higher titanium content resulted in crack blunting, which imparts enhanced toughness. This is consistent with experimental data (see F. Ye, et al.).

www.mse.vt.edu/msewww/faculty/farkas.html; choose "Personal Homepage," then "Atomistic Simulations Laboratory," then "Student Projects."

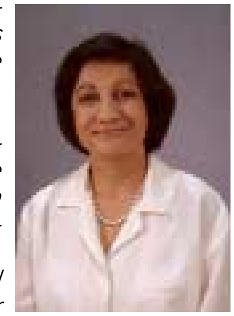
References

Diana Farkas, "Atomistic Studies of Intrinsic Crack-Tip Plasticity," *MRS Bulletin*, [25] 35-38, May 2000.

Robin L.B. Selinger and Diana Farkas, "Atomistic Theory and Simulation of Fracture," *MRS Bulletin*, [25] 11-12, May 2000.

Karen Green, "A New View on Atoms," *NCSA Access*, 1998.

F. Ye, D. Farkas, W.O. Soboyejo, "An Investigation of Fracture and Fatigue Crack Growth Behavior of Cast Niobium Aluminide INtermetallics," *Mat. Sci. & Eng. A*, [264] 81-93 (1999).



Diana Farkas received a bachelor's degree from the Physics Institute "J.A. Balseiro" in Bariloche, Argentina. She completed her doctorate in applied science in metallurgy at the University of Delaware. In 1991, she received a Faculty Awards for Women (FAW) award from the National Science Foundation. She was honored with a Fulbright Scholar Award in 1992, and in 2000 she was named an ASM Fellow.

New MSE Research

Structural Piezoelectric Single Crystal Array Networks (Structural P-Scan); Principal Investigator: S. Kampe; Sponsor: U.S. Army Research Office; $400K; 5/20/01-5/20/04.

Chemically Assisted Ion Beam Etcher for Research in Enabling Semiconductor Process Technology with Application to Novel Photonic and Electronic Devices Based on Group III Nitride and Other III-V Semiconductor Alloys and Heterostructures; Principal Investigator: L. Guido; Sponsor: Air Force Office of Scientific Research; $360K; 3/1/01-3/30/02.

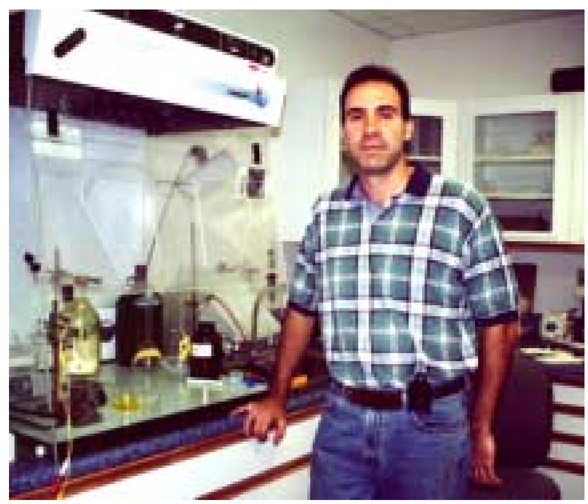
Nano-Mechanical Measurements of Polymer Nanocomposites; Principal Investigator: S. Corcoran; Sponsor: U.S. Army Research Office; $10K; 9/15/01-3/15/02.

Meso-Structural Design of Multiferroic Behavior; Principal Investigator: D. Viehland, J. Li; Sponsor: ONR; $114K; 6/1/01-6/1/06.

Meet Sean Corcoran

LeeAnn Ellis

Sean Corcoran originally planned on becoming a doctor. However, after completing an introductory medical course offered at his high school, and after being advised by doctors to avoid the profession, he turned his thinking toward biomedical engineering and started his undergraduate work at Johns Hopkins University.



Sean Corcoran stands beside his remote AFM/nanoindentation lab facility in Collegiate Square. This lab has been designed to handle electrochemical preparation of single crystals for nanoindentation and atomic force microscopy.

When he realized that this field leaned heavily toward electrical engineering, he began to consider other options. Undergraduate research with Professor Karl Sieradski sparked an interest in materials, and Corcoran wound up with a double major in biomedical engineering and materials science and engineering.

"It's just one of those things," Corcoran said, "probably like most materials people. They don't usually go to school to be materials people; they find it along the way." He remained at Johns Hopkins for his graduate work, completing a master's in 1992 and doctorate in 1994.

From there, he accepted a postdoctoral position at the Naval Research Lab. He worked with Rich Colton in the chemistry division, where he began to specialize in scanning probe microscopy, concentrating on atomic force microscopy and nanoindentation.

He moved into industry for a brief time, taking a position at Hysitron, Inc., in Minneapolis, the company that built the nanoindentor Corcoran used while working at the NRL. As a start-up company, Hysitron was looking for a staff scientist to develop a laboratory.

Corcoran continued page 10

Crystallography in Materials Science and Engineering at Virginia Tech

Maureen Julian

The crystals shown here were grown by students as an exercise in my crystallography laboratory, which is part of MSE 3134, Symmetry and X-ray Powder Diffraction. Copper sulfate pentahydrate was chosen because beautiful, blue, gem-like crystals can be grown from seed crystals in two weeks. The seed crystals were carefully suspended in solution on a human hair. Two temperatures were used—room temperature and refrigerator temperature. Daily growth was monitored by measuring the developing faces.

L.A. Ellis

Large crystal (2.5") grown by Erik Herz (MSE); smaller crystal grown by Stephanie Bryan (ESM)

Copper sulfate pentahydrate is an ore of copper (25% copper by weight). Its mineral name is chalcanthite; it is found in arid regions, often forming stalactic growths on the walls and ceilings of mine tunnels. Historically, it was the first crystal to have its x-ray diffraction pattern taken. This was done in 1912 under the direction of Max Laue, who received the Nobel Prize in 1914 for his proof of the diffraction of x-rays by crystals.

The discipline of materials science and engineering studies the relationship between 1) the structure of matter and its properties, and 2) the modification of those properties by processing and manufacture. On the microscopic scale, structure means crystal structure and electronic and point defect structure; and on a macroscopic scale, structure includes dislocations, grain boundaries and interfaces, polyphase assemblages, and composite materials.

I have developed a crystallography course here at Virginia Tech. Many of my ideas, arrived at independently, are similar to those of Bernhardt Wuensch at MIT. (See "The Teaching of Crystallography to Materials Scientists and Engineers," *Journal of Chemical Education*, **65**, 1988, pp. 494- 501.) It is a junior level course and is integrated with the ceramics course taught by Dr. Carlos Suchicital.

My goals are to give the students 1) access to the crystallography literature, and 2) a working knowledge of x-ray powder diffractometry and its applications to materials science.

The course consists of highly integrated lectures and laboratory exercises. The laboratory exercises include using the Powder Diffraction Files, measuring density by the pycnometer method, growing crystals, using stereographic projections, visiting the crystallography laboratory in Geological Sciences and running powder photographs on their apparatus, understanding x-ray powder analysis, and applying diffraction techniques to various materials science and engineering problems.

The course focuses on two carefully chosen compounds. The first is a "mini" polymer, a small molecule that has both primary (covalent) and secondary (van der Waals or hydrogen) bonding. The structure is simple enough that I can introduce it during the first week of class. I chose hexamethylbenzene (HMB), which is planar except for the hydrogen atoms. This molecule has 12 carbon atoms and crystallizes with one molecule in the triclinic unit cell. The students are introduced to the nonorthogonal world of crystallography, fractional coordinates, and cell constants. Several weeks later, after we complete the portion of the course focused on symmetry, the second compound, which is a framework structure, is introduced. I selected trigonal potassium aluminum disulfate, $KAl(SO_4)_2$), an anhydrous form of alum. By this time in the course, we have made this crystal as a laboratory exercise and have taken its x-ray powder diffraction spectrum during the field trip to the crystallography laboratory in the Geology Department. Framework structures are the crystallographic model structures for both metals and ceramics. In this exercise, the students work with a highly symmetric compound, find special positions, and calculate the volume, density, atomic packing factor, and interatomic distances and bonds lengths.

Reading the crystallographic literature requires knowledge of crystallographic symmetry as found in the *International Tables for Crystallography*. The symmetry section forms the first half of the course. I give a complete and rigorous derivation of the space groups in two-dimensional crystallography. Here we have a manageable set of 10 point groups, 5 Bravais lattices, and 17 planar space groups. For example, for two dimensions, a tree demonstrating the family relationship of subgroups and supergroups within both the point groups and space groups can easily be completed. In three dimensions, with 32 point groups and 230 space groups, these constructions are not remotely possible or even desirable. Another exercise is the construction of Escher-like planar figures with the help of computer programs such as Microsoft Paint. These programs take the tediousness out of paving a two-dimensional space and lead to an understanding of the symmetry operations generated by the act of translating the unit cell.

After we have studied the two-dimensional geometry, the tools are in place for the jump to the third dimension. The student selects a material, either a metal, ceramic, or polymer, and finds its structure in the crystallographic literature. As the course proceeds, all calculations (such as structure factors) are done both on the two study crystals (HMB and $KAl(SO_4)_2$) and the student's own crystal. Special projections along the crystallographic axes are drawn.

Crystallography continued page 11

MSE Gets New Student Computing Laboratory

Diane Folz

As the renovations in Holden Hall continue this year, one of the priorities has been to improve the facilities for undergraduate teaching. The department initiated the new Student Computing Laboratory, a complete computer facility to support the class work of undergraduate students in the department.

"A computer laboratory for our undergraduates was long overdue," said Dr. David Clark, MSE Department Head. "Many of the graduating seniors emphasized the need for such a facility during their exit interviews. Thanks for letting us know!" Five new Dell computers, a printer, and a scanner are now available in 127 Holden Hall to all MSE undergraduate students.

Already, faculty are integrating the computer facility into their classes. Students are able to access specialty software for MSE classes, including Powder Diffraction Database as well as general software listed in the box below. Upon request from the students, Autodesk Mechanical Desktop, a computer cad program, is being installed this month. "It is nice to have computers at our disposal with programs that are on our computers at home," said Pamela Tomlin, a junior in MSE. "These computers allow us, the students, not to waste time going home during the day to work."

Undergraduate Computer Lab Software

Microsoft Windows 2000 Professional	Matlab R12
Adobe Acrobat 5.0	Microsoft Encarta Encyclopedia Standard 2001
Adobe Photoshop 6.0	Microsoft Picture-It Publishing 2001
Adobe PageMaker 6.5 Plus	Microsoft Visual Studio 6.0 Professional
Mathematica 4.1	

Materials Science and Engineering Information Open House

Judy Robinson

The Materials Science and Engineering Information Open House, held on September 24, was a recruiting event designed to entice Engineering Fundamentals students, undecided in their choice of major, to join the MSE Department. Approximately 175 general engineering freshmen attended the event, which began in Hancock Hall with introductory speeches by Dr. David Clark, Dr. Norman Dowling, and Dr. Eric Pappas. The majority of the event was hosted at Holden Hall and included laboratory demonstrations, displays, a poster and information session, pizzas, submarine sandwiches, chocolate, and soda.

The MSE faculty participated by talking with the freshmen and presenting active and interactive demonstrations, and introducing the visiting students to the range of interesting topics available to a materials engineer. The engaging demonstrations included such titles as *Glass Forming, Shape Memory Alloys, Microscopy of Metals and Alloys, Atomistic Computer Simulation of Fracture in Nanocrystalline Iron, The Hot and Cold of High-Tech Ceramics, Materials in Electronics, Sensor Materials and Their Application, Why Does Metal Rust: Fun with Corrosion, Alloy Design and Golf Clubs, and Tension Tests for Strength of Plastics*. The *Night Vision Goggles* interactive display, an annual favorite, was staffed by Tony Salamone, an MSE senior. Also on display were a fireproof suit and a bulletproof vest, providing another example of the importance, and the often-overlooked influence in our everyday lives, of the materials designed and developed by materials engineers.

The overwhelming participation by the sophomore, junior, and senior MSE students played a large part in the success of the evening. The students supported the recruiting effort primarily by talking about their own experiences in the department with the attending freshmen; they mingled with the freshmen and worked the poster session, discussing the concentrations available to materials science majors. Valerie Binetti, a senior, said "…[I]t is important for us, as students, to support recruiting in the college…. The significance of a healthy department not only has an effect on our academic experience, but also on our future."

VMEC Summer Scholars Exchange Program

Robert Hendricks

The Virginia Microelectronics Consortium (VMEC) was created in 1996 to serve the microelectronics industry throughout Virginia. The main goal of the consortium is to facilitate partnerships between industry and academia to address educational, training, and research needs in microelectronics within the state. As a part of fulfilling this goal, the VMEC Undergraduate Scholars Exchange Program offers summer internships at member institutions, which include the College of William and Mary, George Mason University, Old Dominion University, University of Virginia, Virginia Commonwealth University, and Virginia Tech. The program is open to engineering juniors and seniors attending one of these universities and is designed to provide opportunities to participate in research at other Virginia universities and colleges. During the 10-week program, participants collaborate with faculty members and work closely with a VMEC mentor from Infineon Technologies or Dominion Semiconductor in order to gain experience working in a state-of-the-art fabrication facility. Participants receive a $5000 stipend and 3 course credits in microelectronics.

This past summer, I hosted Eddie Bauer, a rising senior in electrical and computer engineering at UVA. Eddie worked with MSE graduate student David Gray and I on optimizing the Virginia Tech Undergraduate Semiconductor Fabrication Laboratory. The lab is designed to provide undergraduate students with hands-on experience in fabricating simple semiconductor devices.

Previous research in this lab has shown that the surface concentration of phosphorous deposited on silicon wafers by solid state sources has an unacceptably high variation across the wafer. This leads to identical devices operating differently, depending on which section of the wafer they were fabricated on. As an introductory exposure to undergraduate students, it is important that the process allow students to create working devices without non-ideal effects. By examining the effects of modifying the pre-deposition step, and using SIMS and sheet resistivity measurements (graciously performed by Greg Fitzgibbon and Rob Johnson of Dominion Semiconductor), Eddie's goals were to identify the parameters required to make uniform devices and to model the time and temperature dependence on the concentration and diffusion profile of phosphorous in silicon.

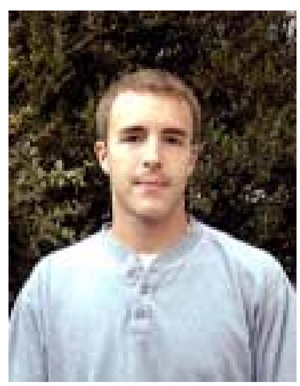
Courtesy R. Hendricks

Eddie Bauer (ECpE, UVA) places a silicon wafer in a diffusion furnace.

A second aspect of Eddie's research was to examine spin-on doping in collaboration with Drs. M. Jhabvala and C. Allen of NASA Goddard, where ion-implantation is used to create radiation detector preamplifiers. This technique creates defects in the crystalline structure of the silicon. At the milli-Kelvin temperatures of space, these defects cause a low-power amplifier to have excessive noise. Phosphorous spin-on or solid-state diffusion are alternate methods of doping which should produce fewer defects but may not be as uniform as ion-implantation. Eddie worked on comparing the spin-on process and the solid-state process to determine which doping parameters provide the most uniform material. The goal was to provide NASA Goddard with enough information to determine whether spin-on or solid-state doping are viable substitutes for ion-implantation.

VMEC Undergraduate Scholars Exchange Program: Carbon Nanotubes for Field Emission

Andrew Signor



This summer I had the wonderful opportunity to participate in the VMEC Undergraduate Scholars Exchange Program. As a representative from the Virginia Tech Materials Science and Engineering Department, I spent the summer studying the synthesis of carbon nanotubes (CNTs) for field emission applications at the Electrical and Computer Engineering Department of Old Dominion University in Norfolk. I worked closely with Dr. Weihai Fu, a postdoctoral researcher at ODU, in developing a gated CNT emitter and optimizing the microwave-plasma-enhanced chemical-vapor-deposition synthesis of CNTs on such a device.

CNTs were first synthesized in the early 1990's[1] and have been observed to possess many novel properties. The wide range of CNT applications includes hydrogen storage, probes for scanning probe microscopy, structural composites, field emission displays, and molecular electronics.

Simply put, CNTs are nanoscale hollow cylinders whose walls are composed of graphitic carbon layers. CNTs have been synthesized in many different forms, varying in their overall size, number of walls, and chirality (wall orientation). Many different properties (mechanical, electrical, and chemical) have been observed to be dependent on the CNT structure variables just mentioned, and much of the present research is devoted to selectively growing CNTs with specific properties. One of the most utilizable properties of CNTs is the field emission property: the ability to emit electrons while under the influence of an electric field. In many cases, the field emission properties of CNTs have been proven to be much more desirable than conventional electron emitting materials. Field emission properties may be applied to areas such as flat panel display technology and scanning electron microscopy

VMEC continued page 8

Student and Alumni News

Global Hokies

LeeAnn Ellis

Environmental Policy in Europe

Lisa Copley and Sam Allin, both MSE juniors, spent the summer in Europe learning about environmental measures underway in several areas. Sam and Lisa were the only engineering students among a group that included students from animal science, political science, agricultural economics, forestry, and business. They traveled to Europe as part of the Undergraduate Interdisciplinary Environmental Summer Semester, sponsored by the University Office of International Programs (UOIP). The purpose, as outlined in the UOIP website, was to provide "an interdisciplinary international environmental educational experience" through a comparison of economic and environmental policies of European Union countries and the United States. The program ran from May 22 to August 12, and students could earn up to 14 credits.

Both Lisa and Sam are pursuing a concentration in Green Engineering, defined in the Virginia Tech College of Engineering website as "environmentally conscious attitudes, values, and principles, combined with science, technology, and engineering practice, all directed toward improving local and global environmental quality."

"It's why I got into engineering in the first place," Lisa said. "I want to make products that are good for the environment, and materials science and engineering seems to go along with that."

The students toured a power plant in Sweden, wind turbines in Denmark, an experimental sustainable community in Germany. In England and Ireland, they visited agricultural sites, where Sam says he gained a new respect for those in agricultural majors.

"What impressed me most," said Sam, "was the attitude towards sustainability and recycling." He defined sustainability as providing for the needs of today without sacrificing resources needed for future generations. In particular, Sam was impressed with Stockholm's high efficiency power plant located in the middle of the city.

"There was a great deal of environmental planning in the community," Lisa said, speaking of their visit to Stockholm. "I was impressed that they recycle up to 32 types of materials," and everyone is encouraged to maintain a compost pile for food scraps. Lisa also praised the European system of mass transit, where buses, trains, and subways offer environmentally friendly and efficient transportation to most cities and towns across the continent.

Materials Engineers can play a key role in preserving the environment for future generations

Courtesy Sam Allin

Sam (far left) and Lisa (far right) tour Roman ruins with other Environmental Studies students.

Sam talked about gas prices and the fact that U.S. prices are heavily subsidized. In Europe, pollution and gas consumption translate into a "social cost up front," he explained, "so that people who consume the gas are paying for it…the polluter pays rather than society."

"Europe is ahead of us with environmental awareness," Lisa said. "They had to be aware earlier than we did because we're a large country; we have a lot of new land with a lot of new resources." So we haven't had to face the problem of a shortage of resources as early as they have. We've had a delayed reaction."

Sam and Lisa both found many areas for materials applications and opportunities for a materials engineer to contribute to ongoing efforts to protect the environment and provide comfortable living for citizens. "Everything goes back to materials and what you use to make something, whether it's green or not," Lisa observed.

Aside for concentrating on environmental concerns, they found other interesting ways to spend their free time. Virginia Tech maintains the Center for European Studies and Architecture (CESA) in Riva San Vitale, Switzerland, which served as the base for this summer program. Sam, a mountain biker and runner, named the Swiss Alps his favorite spot on this tour. He spent time running in the Alps and participated in the Swiss Alpine Marathon, a run of 26 miles through the snow-capped Alps, finishing a respectable 122 out of 1000.

The trip also offered unique opportunities for the students to acquire new insights into how social issues besides the environment are handled. Sam observed that there are different ways to approach social issues such as drug use or prostitution. "Maybe certain things aren't a crime," he said, but rather a social condition that must be either remedied or perhaps accommodated.

Looking back on her experiences as she returned to Virginia Tech this fall, Lisa recalled the many applications for materials engineering that she observed. "Transportation, wind turbines, power plants, right down to the actual building materials people use to make things sustainable. I can feel a huge explosion in materials science and engineering in the future," she said, once the United States catches up with Europe in environmental concern.

A Year in Australia and Switzerland

An opportunity to see a new part of the world and to explore a different perspective of the United States were two motives that prompted **Erik Herz** to travel to Australia and Switzerland last year. From July to December 2000, Erik attended Monash University in Melbourne to study polymers, biomaterials, and economics. Then from January to May 2001, he studied classical history and Italian at CESA in Switzerland.

In terms of materials education, Erik found that the approach at Monash University concentrated heavily on processing. As a country, Australia has roughly the same landmass as the United States, but at 18 million people, it has less than a tenth of the population. "They have a very large materials resource base, so a lot of their materials teaching is based on processing, on getting the material out of the ground and making it useful to somebody." In the United States, Erik explained, we are looking more at how to refine certain materials or how to create new ones.

One aspect of teaching that impressed him was the manner in which theory was introduced. "We would be taught theory one day, and the next day we were taught how that theory is applied," linking theory to real life.

An introductory course in biomaterials particularly caught his interest. "The field exists such that it's there to help people, it's there to accommodate different people," he explained. "Body chemistries vary, so you have to tailor everything


Courtesy Erik Herz

Erik, far right, inside the Colosseum in Rome with members of his International Studies group.

that you do to the individual." Even teeth, which can be mass-produced as blanks, still require reworking for each individual.

Erik was able to fulfill a lifelong dream by attending the 2000 Summer Olympics when he and three other students rented a Mitsubishi station wagon, which served both as transportation and hotel for six days of events in Sydney.

Another dream was realized in Italy with a visit to Pompeii, a city buried in volcanic ash 2000 years ago. The city was so well preserved that it now "allows us very poignant glances into daily life" as it was. "It's very materials oriented," Erik said, "in how these materials have survived," such as mosaics that made up the floors of buildings and original graffiti found on the walls.

This fall, Erik returned to Virginia Tech to begin his junior year. He is working toward a triple major in materials science and engineering, economics, and international studies. His work at Monash University helped to expand his materials interests to include polymers and biomaterials. He would like to find a way to combine these interests, along with electronic materials, and he has recently begun research with the Optical Science Engineering Research Group that involves all of these materials areas.

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More Student & Alumni News

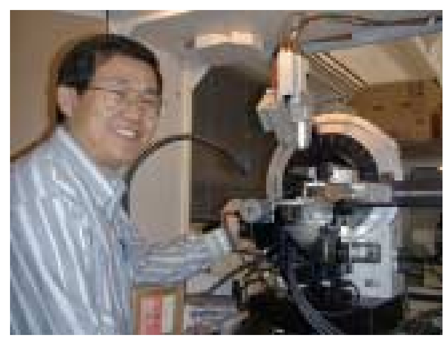
In June, **Charlie French** presented a paper at the IEEE 14th Biennial University/Government/Industry Microelectronics Symposium held at VCU's School of Engineering in Richmond, Virginia. "Determination of Junction Depths for Phosphorus Diffused in Silicon" developed from his MSE senior design project, a team effort between Charlie, **Dave Belman** (MSE '01), and **Dave Kardes** (MSE '01).

Charlie worked with Dr. Robert Hendricks to expand and revise this project into a paper for the conference. The paper summarizes work done to characterize the diffusion process of pn junctions and n-wells for MOSFETS. Charlie is currently working for Haleos, Inc., in Blacksburg as a CVD (Chemical Vapor Deposition) co-op. He will complete his undergraduate degree in MSE next spring. ❖

Celine Mahieux (MESc '97) joined Alstom Power in September as the manager for R&D materials at their Hydrogenerator Technology Center in Birr, Switzerland. Celine writes, "I view hydrogenerators as a great opportunity to further develop the use of composite materials (polymer-based and metal) for large non-aerospace applications." ❖

Bob Baoping He (MESc '92) received an R&D 100 Award for 2001. This award is presented annually by *R&D Magazine* to the 100 most significant inventions. Previously recognized inventions include automatic teller machines (1973), the halogen lamp (1974), the fax machine (1975), and HDTV (1998). Dr. He, as a principal developer, received this award for the "D8 DISCOVER with GADDS for Combinatorial Screening," a two-dimensional x-ray diffraction system designed for rapid material screening.

This invention was developed at Bruker Advanced X-ray Solutions (AXS), where Dr. He is the XRD and Mechanical Engineering Manager, responsible for research and development in x-ray diffraction, management of the mechanical engineering division, and product management for several products. Bruker AXS is a leading provider of advanced x-ray solutions worldwide for life and advanced materials sciences, headquartered in Madison, Wisconsin, with facilities in the U.S., Germany, and the Netherlands.



Bob Baoping He, R&D 100 Award recipient for the D8 Discover designed for rapid material screening.

Bob completed his Ph.D. in materials science and engineering in 1992 at Virginia Tech under Dr. Charles Houska. Until 1995, he held a postdoctoral position under Dr. Guo-Quan Lu and Dr. Robert Hendricks in the MSE Department. ❖

Richard Hudgins (MSE '96, MEng. '98) has taken a position with Marion Composites in Marion, Va., as an F-22 Project Engineer. Marion Composites is under contract with Lockheed Martin to build 28 parts for the F-22 Raptor, an Air Force

Alumni news continued page 9

VMEC continued from page 5

(SEM) electron sources. A commercially available Field Emission Display (FED) has been produced using CNT technology.[2]

The combination of the enormous aspect ratio of CNTs (diameter on the order of nanometers, length on the order of microns) and their electronic structure gives them superior field emission properties. An applied electric field becomes significantly enhanced near the CNT tip due to their geometry. This field enhancement allows electrons to be emitted from the CNTs under the influence of a relatively modest macroscopic field. While the field enhancement at the CNT tip is significant, the macroscopic field needed to induce electron emission is still large enough to inhibit high-frequency operation of such devices. For this reason, we were interested in developing a gated CNT emitter in which a relatively small gate field superimposed on a larger background field is used to control electron emission. We were successful in developing a gated device in which a gate field of about 50V influenced electron emission from the CNT cathode, thus allowing the possibility of high-frequency operation.

This experience has exposed me to cutting-edge materials science research and has also ignited my interest in pursuing a graduate degree in the exciting field of materials science applied to microelectronics.

1. Ijima, Sumio, "Helical microtubules of graphitic carbon," *Nature*, **354** [7] November 1991.

2. Choi, W.B., et al, "Fully sealed, high-brightness carbon-nanotube field-emission display," *Applied Physics Letters*, **75** [20] 15 November 1999.

Andrew Signor is a senior in the Materials Science and Engineering Department at Virginia Tech. He is making plans to attend graduate school and to focus on microelectronic materials.

Other Department News:

The new **Center for High Performance Manufacturing** was launched in July with $4.35 million in state funding and matching funds from universities and equipment manufacturers. The effort to establish the center was led by Virginia Tech's College of Engineering and James Madison University's College of Integrated Science and Technology (ISAT). Faculty across the College of Engineering will be involved with the center, including **Alex Aning** (EF, MSE) and **Carlos Suchicital** (MSE). **Ron Kander**, who was appointed adjunct professor in the MSE Department after leaving Tech to become the department head for ISAT at JMU, will serve as an associate director.

The mission for this new center is to help manufacturing firms (especially in Virginia) become high-performance manufacturers via research and development of enabling tools and technologies and the successful transfer and implementaiton of these items. ❖

Guo-Quan Lu is on sabbatical at NASA/Goddard Space Flight Center this semester. He is working with scientists and engineers in the Detector Systems Branch, where several projects are underway in the areas of design, fabrication, and testing of Micro-Electro-Mechanical-Systems (MEMS) for detectors in space telescopes and satellites. "The mission of these projects is to expand knowledge of the earth and its environment, the solar system, and the universe through observations from space." Dr. Lu is helping to develop integration and packaging ideas, and concepts for the MEMS-based detector systems. Packaging is particularly challenging for these detectors, which face cryogenic temperatures below 40°K. ❖

Alex Aning traveled to Ghana this summer, where he visited three major universities to talk with faculty and students about the Virginia Tech MSE program. He is already in contact with two students who are interested in applying for fall 2002 admission. He met with faculty and students in physics, materials science and engineering, metallurgy, mechanical engineering, chemical engineering, and chemistry at the University of Cape Coast (Cape Coast), Kwame Nkrumah University of Science and Technology (Kumasi), and the University of Ghana (Legon). ❖

Guo-Quan Lu traveled to China over the summer to present a paper at an international conference held in Beijing. While there, he met several students from the MSE Department at Hsinghua University, from which we receive many applications. He currently has two graduate students from Hsinghua. ❖

Bill Reynolds has been named Assistant Department Head for MSE. Reynolds is devoting a great deal of time to the MSE graduate program, which is expected to see significant growth in coming years. **Susette Sowers** has been appointed graduate coordinator to assist Dr. Reynolds. ❖

Diane Folz attended the 8th International Conference on Microwave and High Frequency Heating in Bayreuth, Germany, September 3-7. She participated in a short course taught by Ricky Metaxas, an expert in the field of microwave heating. During the conference, Diane spoke with a number of potential graduate students who would like to continue their microwave processing studies in the U.S., and she also initiated discussions with Dean Monika Willert-Porada about collaborative funding for an exchange program for students in this technology area. The organizers of the 3rd World Congress on Microwave and Radio Frequency Processing held planning meetings for the upcoming Congress, scheduled next September in Sydney, Australia. ❖

Brian Love will begin a five-month sabbatical in January. He will be working at the National Institute of Standards and Technology (NIST) in Gaithersburg, Maryland. The Materials Science Group is divided into six subclasses of materials research, and Dr. Love will work in the dental materials section on development projects. In addition, he will spend about a month working at Wake Forest in Winston-Salem, North Carolina, where he will help to establish the new School of Biomedical Engineering and Sciences, which will be operated jointly by Wake Forest and Virginia Tech. He will be one of the early links between the two universities, and he will have an opportunity to learn more about where his research can be applied. For more information about this joint venture, go to: *www.technews.vt.edu/Archives/2001/Oct/01405.html.* ❖

Introducing Materials Science and Engineering to C-TECH^2 Participants

By Grace Tran

The Office of Minority Engineering annually sponsors C-TECH^2: ***C**omputers and **Tech**nology at Virginia **Tech***, a summer program for rising junior and senior women currently enrolled in Virginia high schools. The 3-week program allows students to explore applications of engineering, math, and science through hands-on activities. I became involved in the program as an instructor because I wanted to increase the interest of young women in the engineering field and expose them to the diverse applications of materials science and engineering.

The program consisted of 50 students who were divided into two groups during the activities. Upon introducing MSE to the young women, many were not even aware that such a discipline existed! Feeling disheartened for only a few seconds, I was able to define MSE simply by remembering Dr. Kander's words: "Materials is the study of STUFF!" I was excited to have Diane Folz demonstrate the thermal properties of space shuttle tiles and the Meissner Effect in superconducting materials. She caught the attention of the students by heating one side of the ceramic tile with a blowtorch to elevated temperatures and inviting volunteers to touch the other side of the tile with their bare hands. Additionally, students were in awe when liquid nitrogen was used to show the transition of a material from the normal to superconducting state, otherwise known as the Meissner Effect.

Following her demonstrations, I planned for the students to perform an experiment involving super-absorbent polymers in…disposable diapers!

The students formed small groups and were given a diaper of either premium-quality or low-quality. They had to isolate and measure the amount of superabsorbent polymer in a disposable diaper and study how well the polymer absorbed varying types and concentrations of aqueous solutions. Some groups were more successful than others, especially in having to fluff the core padding of the diaper to separate the polymer granules. One group perfected their technique so well, they were able to extract more polymer granules from the generic brand than those working with the national brand!

The students also showed great interest during the experiment when they were determining the capacity of the diapers; 1% solution of NaCl was used to simulate urine. Both the national and generic brands were determined to hold approximately 400g of the solution, a weight that babies may not want to carry on their bottoms! Diane Folz commented on the cost difference between the two brands although both diapers performed relatively the same.

I find C-TECH^2 to be an excellent opportunity for both high school students and college students like myself. The program allowed the younger students to learn about the different engineering disciplines at Virginia Tech and thus enabled them to become familiar with the wide applications of materials science and engineering. As a college student, I faced the many challenges involved with teaching, such as preparing the lessons, researching the background information, and obtaining the needed materials for the experiments. I thoroughly enjoyed the experience, as the teaching process allowed me to reinforce a lot of what I learned as an undergraduate. I also had the pleasure of working with Diane Folz and welcome the opportunity for similar experiences in the future as a graduate student at Virginia Tech!

Grace Tran completed a B.S. in MSE at Virginia Tech this past spring. In September, she entered graduate school, also at Tech, in the Department of Industrial Systems Engineering, where she hopes to incorporate her MSE knowledge with her interest in Human Factors Engineering.

Alumni News continued from page 7

fighter jet just going into production. Ric and his wife, Merrill, have 2 children, Rachel, 3, and Richard, Jr., 1. ❖

Drew Galloway (MSE '97) and Trudy Ann Scholten were married June 29. Drew is a materials engineer with TDA Research, Inc. in Golden, Co. He recently received two grants to develop a technique of field welding silicon carbide composites. Trudy, a chemical engineer, also works for TDA Research. ❖

Beth Oborn (MSE '98) married Matt Robinson (ENGL '00) June 10, 2000. Beth completed her Master's in materials science and engineering at the University of Florida last December. She is a Research Chemist at Bostik Findley near Philadelphia. ❖

Mike and Becky Stawovy (both MSE '91) are the proud parents of a second son, Samuel Valentine Stawovy, born September 27, 2001. Samuel weighed 7 lbs. 14 oz, and was 27.75" long. ❖

London to Singapore: fromRussian newspaper

Scott Zentack (MSE '94) is in the middle of a "Bicycle Odyssey" that began in England in June with plans to ride through 20 countries, ending up in Singapore. ❖

Robert Carter (B.S. '93, M.S. '97, Ph.D. '01) began a post-doc position in November at the Army Research Lab in Aberdeen, Maryland. ❖

People in Materials

Meet Sarah Smith (MSE '01)

LeeAnn Ellis

With a chemical engineer father and a mathematician mother, it's no surprise that Sarah Smith did well in math and science in high school. When the time came to think about college, she decided engineering would be a good way to combine these two strengths. Virginia Tech proved to be an ideal choice with its many engineering options, reasonable tuition, and the added bonus of being a workable distance from her home, which is near Pittsburgh, Pennsylvania.

As far as choosing which engineering field to study, Sarah said, "I thought about chemical engineering, but I came to an information session where I decided that [materials science and engineering] was more applicable to real life."

Along the way, she gained experience through a summer internship with Elizabeth Arden Manufacturing in Roanoke, Virginia. She found that the internship was "a good place to start," offering an opportunity to find out something about real world engineering. She also spent her last two years at Tech serving as an engineering tutor for the Minority Engineering Program, where she worked with students at varying academic levels and abilities. Last fall she was awarded the Alfred Knobler Scholarship, and she was also a recipient of a Virginia Tech Scholar Scholarship during each of her four years here.

Aside from technical matters, Sarah is an avid swimmer and, in general, loves the outdoors. Following graduation, she and her sister, Ellen, embarked on a nationwide trek to see the United States, a trip she describes as amazing. "We visited 27 states, 10 national parks, countless state parks, and drove 10,000 miles in 5 weeks!" They camped out most nights and occasionally stayed in youth hostels. Her favorite stop was Yosemite Park, with the Badlands and Montana running a close second.

Sarah (left) and her sister, Ellen, along the California coastline, May 2001

Sarah is not certain where her future lies. Somewhere down the road, she would like to find a way to combine her love of the outdoors with a career. In July, she joined BWX Technologies in Lynchburg, Virginia. The company does work for the U.S. Navy, making nuclear reactors for aircraft carriers and submarines. As a process engineer, Sarah is responsible for production of the nuclear cores. So far things are going well, and she is enjoying Lynchburg, which she describes as a small town with a lot to offer.

Corcoran continued from page 2

After a year and a half, he'd had enough of industry life and turned back to academia, the career he had in mind all along. He joined the faculty at Virginia Tech in 1998.

He credits his industrial experience with giving him a boost in his research endeavors. This exposure provided him with many connections in industry and helped him become familiar with the types of problems seen in industry and how people approach research in an industrial setting.

He is currently involved in several projects, most recently with the Army Research Lab in Aberdeen, Maryland, where "Alex Hsieh is very interested in mechanical properties of nanocomposite materials used, for example, in helicopter canopies." Specifically, Corcoran is involved in nanoindentation testing to determine the ballistic impact properties of these materials.

He is also working on a larger project involving nanoporous metals. Interest in this subject originally focused on understanding the formation of nanoporosity, which is a result of certain corrosion processes. A nanoporous metal, Dr. Corcoran explained, "is basically a material that looks very much like a sponge," with pores that are interconnected. The material is about 30% metal and 70% open space, and applications for such a material range from special filtration needs to sensor technologies.

"This process is old," Corcoran said. "It has been studied in the corrosion literature because it leads to cracking." However, a handful of researchers are taking another look from the viewpoint of possible applications. Dr. Corcoran has been looking into using nanoporous platinum for cardiac pacing. The National Science Foundation funded this research during the early, fundamental stages, where studies have been done to determine how the materials are formed and how the pores, once formed, can be manipulated.

In the classroom, Corcoran describes his teaching style as laid back. "I tend to let things flow, depending on how the class is going." He stresses the basics and encourages students to understand the problems rather than just solving for answers. He asks a lot of "why" questions in such courses as "Elements of Materials Engineering," "Kinetics," and "Structures of Materials." He's more interested, he says, in how students approach answers than what the answers actually are. "To me, the answer is not so important. I want to make sure they're thinking appropriately." Corcoran differentiates between training and education. Rather than train students to solve problems, "I focus more on educating them to think so that they can solve problems that they've never seen before."

Sean and wife, Amy, are parents to 21-month-old William, and they are expecting a second child next spring. Aside from his engineering interests, Sean says, parenting is what he does, along with an occasional mountain biking expedition with his graduate students.

Crystallography continued from page 3

These two-dimensional projections are members of the 17 planar space groups. The students' efforts culminate in a four-minute oral presentation and a term paper.

The oral presentations are one of the highlights of this course. Each student is required to present a crystal structure to the class. A specific format is given in order to standardize the presentations, to insure the rigor of analysis, and to allow each person to compare work to a peer's work. The term paper benefits greatly from this group exposure. After the oral presentations, the student writes a term paper, comparing the student's own crystal structure with HMB and $KAl(SO_4)_2$. A peer review is done.

In the second part of the course, x-ray powder diffractometry is explored. Topics include indexing cubic and hexagonal structures, measuring precise lattice parameters, determining a phase diagram, understanding long-range order, calculating crystalline size and lattice strain, and finally quantitative analysis of mixtures of powders. The Powder Diffraction Files are used to identify the student's own crystal as well as for the identification of single and multiple phase unknowns. Additionally, students generate an Excel spreadsheet of the spectrum for their own crystal and compare it to the spectrum found in the PDF.

Special thanks in the development of this crystallography course goes to Dr. Carlos Suchicital, the MSE 3234 classes in both 2000 and 2001, Dr. Norman Dowling and Dr. David Clark for enthusiasm for the development of the laboratory exercises, to Dr. Ross Angel for demonstrating diffraction apparatus, to Dr. Nancy Ross for her support, and to everyone else who helped.

Maureen Julian received her Ph.D. at Cornell University specializing in the crystallography of the chelates. She was a research fellow at University College London with Dame Kathleen Lonsdale who did the crystal structure of HMB and who edited the early editions of the International Tables for Crystallography. Before coming to Virginia Tech, Maureen Julian was a research scientist at the Nuclear Weapons Laboratory at Kirtland Air Force Base in Albuquerque, New Mexico. At present, she is writing a text from material developed in this course.

Recent MSE Publications

E.C. Pappas, R.W. Hendricks, and J. Franks, "Satisfying the Non-Technical ABET "a-k" Requirements: The Virginia Tech Materials Science and Engineering Communications Portfolio," *Proceedings*, 2001 ASEE Southeast Section Conference.

C.S. French, D.P. Belman, D.E. Kardes, and R.W. Hendricks, "Determination of Junction Depths for Phosphorous Diffused in Silicon," *Proceedings*, 14th IEEE Biennial University/Government/Industry Microelectronics (UGIM) Symposium, Richmond, Va., June 17-20, 2001.

D.S. Myers, J.L. Meyer, P. DePasquale, and R.W. Hendricks, "An Interactive Program for Determining Junction Depths in Diffused Silicon Devices," *Proceedings*, 14th IEEE Biennial University/Government/Industry Microelectronics (UGIM) Symposium, Richmond, Va., June 17-20, 2001.

P.D. Eckerman and R.W. Hendricks, "Wafer Traveler Design for an Undergraduate Microchip Fabrication Facility," *Proceedings*, 14th IEEE Biennial University/Government/Industry Microelectronics (UGIM) Symposium, Richmond, Va., June 17-20, 2001.

B. Gaffey, L.J. Guido, X.W. Wang, and T.P. Ma, "High-Quality Oxide/Nitride/Oxide Gate Insulator for GaN MIS Devices," *IEEE Transactions on Electron Devices*, Special Issue on Group III Nitride Electronics, **48** [3] (2001).

N.B. Rex, R.K. Chang, and L.J. Guido, "Threshold Lowering in GaN Micropillar Lasers by Means of Spatially Selective Optical Pumping," *IEEE Photonics Technology Letters*, **13**, 1-3, (2001).

G.Q. Lu, "3-D, Bond-Wireless Interconnection of Power Devices in Modules Will Cut Resistance, Parasitics and Noise," *PCIM Power Electronic Systems Magazine* **26** [5] (2000).

K.L. Droesch, B.J. Love, and V.M. Vaubert, "Characterization of Water Inhibition in Light-Cured Dental Resins," *Biomaterials Engineering and Devices, Human Applications*, **2,** 61-65 (2000).

D. Farkas, "Fracture Mechanisms of Symmetrical Tilt Grain Boundaries," *Phil. Mag. Lett.*, **80** [4] 229-237 (2000).

Exploring Materials
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On the Cover (Border)
Micrograph of individual crystals of titanium diboride (TiB_2) produced in-situ within a near-gamma titanium (Ti47Al) matrix by reaction synthesis. Courtesy Raphael Martin (M.S. '94) and Steve Kampe.

Head's Up

David Clark

I am pleased to report that our department is in great shape and getting better! We have just completed a visit from the Accreditation Board for Engineering and Technology (ABET). This is the first time that the undergraduate program has been evaluated under the new EC 2000 rules that require a continuous assessment component. Although we will not know the official outcome until next year, our visitor found no deficiencies or weaknesses. We appreciate the hard work of the faculty and staff in getting us ready for the visit and are especially grateful to Professors Steve Kampe, Eric Pappas, and Ron Kander, and the rest of the ABET Committee (Jan Doran, Jessamyn Franks, LeeAnn Ellis, and Judy Robinson) for leading the efforts.

Our academic records office has been restructured to accommodate the growth of the graduate program. Jan Doran will continue to provide coordination and academic services for the undergraduate students. A new office of graduate studies has been established under the direction of Professor Bill Reynolds (recently appointed as assistant department head). Professor Reynolds, with the assistance of Susette Sowers, will focus on recruitment, increasing the selection of graduate courses, and expanding our distance learning program.

Our faculty continues to be successful in competing for research dollars. Several federal agencies, including ONR, NSF, ARO, and NASA recently have awarded contracts to our faculty. Private industry and the State of Virginia, through its Center for Innovative Technology, are also supporting research. These contracts will play a critical role in building our graduate program.

We have received over 300 applications for our three open faculty positions. Professor Norman Dowling and his committee are screening the applications so that potential candidates can be invited to campus for interviews in the near future. We hope to fill these positions by the start of the Fall Semester.

The department is doing its part to help the university realize the goal of getting into the top 30 by 2010. In order for this to occur, the College of Engineering must move into the top 10 and, likewise, MSE must increase its ranking significantly. To meet this goal, we are participating in college initiatives to create the Virginia Tech Institute for Critical Technologies and a School of Biomedical Engineering. The latter is a joint venture between Virginia Tech and Wake Forest. You will be hearing more about these initiatives in future newsletters and special news releases.

Several labs and the main office complex have undergone renovations since January. A new undergraduate computer lab also has been added. These changes have made MSE a more "user friendly" and safer place to learn and work. Other facilities modifications and equipment acquisitions are in progress.

In closing, I wish to thank the faculty, staff, advisory board members, students, alumni, and college administration for their strong support during my first 10 months on the job. With your continued support, MSE will prosper and fulfill its vision to be recognized internationally for:

- Providing outstanding, state-of-the-art undergraduate and graduate education, and
- Conducting cutting edge, visionary research in materials.

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