Penn State is a major, comprehensive research university. It counts among its faculty many leading scientists and scholars and ranks among the top universities in terms of research funding obtained from government and industry.

Graduate study in materials science and engineering is centered at the Penn State University Park campus—the largest and the original campus in a system that spans the Commonwealth. More than 39,000 students are in residence at the University Park campus, which is located in the town of State College, at Pennsylvania’s geographic center. The surrounding Allegheny Mountains provide beautiful scenery and many opportunities for outdoor recreation, including biking, hiking, water sports, skiing, and picnicking.

Penn State offers all the facilities of a major university and a full calendar of lectures and other academic events. In addition, the Center for the Performing Arts brings professional musical, theatrical, and dance productions from around the world to campus. Other campus organizations sponsor a wide range of cultural events, and the Palmer Museum of Art hosts a range of exhibitions.

The University has outstanding recreational facilities and programs, including many intramural sports activities: softball, basketball, football, volleyball, and others. Penn State football brings thousands of alumni and fans back to Beaver Stadium each fall. The newly erected Bryce Jordan Center is the site of Nittany Lion and Lady Lion basketball, as well as a center for concerts, athletic tournaments, and cultural events.

The University Libraries have holdings of about 3.6 million volumes with on-line catalog access. The central Pattee Library is supplemented by specialized satellite libraries, including the College of Earth and Mineral Sciences Library in Deike Building.
The Department of Materials Science and Engineering at Penn State, as currently organized, was formed in 1967. Its evolution, however, was unlike most such departments across the country that were initiated and dominated by one of the classic materials science disciplines. At Penn State, the Department of Materials Science and Engineering has its roots firmly planted in the College of Earth and Mineral Sciences—a college with an established tradition in mineralogy and earth sciences. Strong academic programs were established in metallurgy in 1967–68 and in ceramic and mineralogy in 1973. Science, another subject with a rich history at Penn State, was first offered as a major in 1934. These three disciplines were the nucleus of the newly formed department in 1967. The addition of the Polymer Science program in 1972, and the interaction with the multidisciplinary Intercollegiate Graduate Program in Materials, completes what is today one of the finest and best-balanced departments of materials science in the country. A recent study by the National Research Council ranked the department among the top ten materials science departments in the nation.

The department offers graduate degrees (M.S. and Ph.D.) in materials science and engineering with specialties in ceramic science, fuel science, metals science and engineering, and polymer science. An interdisciplinary graduate program, the Intercollegiate Graduate Program in Materials, is administered through the Graduate School.

The department is large and diverse, affording students the opportunity to interact with faculty and with postdoctoral and graduate students from a wide spectrum of disciplines. There are forty full-time faculty members, some 200 graduate students, and about 175 undergraduates currently in the department.

Materials science courses cut across disciplines, and add to those in the principal science. Students are encouraged to broaden their horizons by taking these and other University-wide courses.

Faculty members in the Department of Materials Science and Engineering have many responsibilities, including teaching and advising students, undertaking research and disseminating results, maintaining academic standards, and performing other services for the University. Many also participate in research projects in the various cross-disciplinary centers such as the Center for Advanced Materials, the Materials Characterization Laboratory, the Energy Institute, the Intercollegiate Materials Research Laboratory, and the Electronic Materials and Processing Research Laboratory. Several materials science faculty members have been appointed to the Materials Research Institute Advisory Board, the umbrella coordinating group for materials research at Penn State.

Students and alumni have consistently rated the faculty above average in teaching. Eight of the current faculty have won university-wide teaching awards. The faculty's research productivity is outstanding, as measured by the national and international recognition of their peers, the number and quality of papers published, and the amount of research dollars generated (nearly $12 million in outside funding in 1995–96).
General Admission Requirements for the Graduate Program

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All graduate programs in the department have many more applicants each year than can be accommodated. Usually, 40 to 100 people apply for each opening. No general criteria will guarantee admission. Only the best-qualified applicants are admitted for each opening depending on the number of openings available and the compatibility of students' interests with current research projects.

Applicants must have received, from an accredited institution, a baccalaureate degree earned under residence and credit conditions substantially equivalent to those required by Penn State. No fixed minimum grade-point average (GPA) is required for admission, but a junior-senior grade-point average of at least 2.50 on the scale of A (4.00) to D (1.00) is recommended by the Graduate School. Most incoming students have a GPA of at least 3.00.

Scores on the Graduate Record Examination (GRE)—verbal, quantitative, and analytical—are no longer required by the Graduate School for completion of the admission process. However, all students, especially those from foreign countries, are strongly advised to submit GRE scores with their applications. In many cases, the GRE is the only common factor that can be used to compare applications of similar merit.

The general graduate admission requirements are stated in the General Information section of the Graduate Degree Programs Bulletin. Application forms for admission are sent out by, and should be returned to, the department at the address that appears above. Applicants also should arrange for two or three letters of recommendation to be sent to the same address. Copies of academic transcripts need be sent only to the Graduate School.

Most students admitted to our graduate program are offered financial assistance in the form of research or teaching assistantships. For the 1996-97 academic year, these paid between $14,000 and $15,000 for two semesters plus the summer session, with all tuition paid.

Students who wish to apply for graduate studies in the Department of Materials Science and Engineering should contact the graduate program coordinator at the address above.
The Ceramic Science specialty covers a wide field with special emphasis in ceramic processing, physical ceramics, chemical ceramics, and glass science. Special facilities exist for research in areas of electroceramics, phase equilibria, mechanical properties, thermal properties, surface characterization and properties, high-temperature reaction kinetics, coatings and thin films, solid-state synthesis, dielectric and ferroelectric materials, corrosion studies, and composite materials.

FACULTY
Paul W. Brown, Professor of Materials Science and Engineering, B.S., M.S., Ph.D. (Wisconsin)
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Long-Qing Chen, Assistant Professor of Ceramic Science and Engineering, B.S. (Zhejiang Univ.), M.S. (SUNY), Ph.D. (MIT)
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Gory J. Green, in Charge of Graduate Option

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Fuel Science (FSC)

The Fuel Science program at Penn State provides advanced learning and research opportunities in the science and engineering of energy and fuel use. The program has traditionally emphasized the major fossil fuels (coal, oil, and natural gas), but biomass and other renewables are playing an increasingly important role in the curriculum.

The focus of fuel science is the conversion of fuels into usable energy and value-added products. Advanced fuel formulations, energy efficiency, and environmental aspects of fuel use dominate the research agenda. Pollution prevention and abatement are high priorities. Specialized facilities exist for the chemical and physical characterization of liquid, solid, and gaseous fuels, the conversion of fuels from one form to another (carboxylation, liquefaction, pyrolysis, petroleum processing), the production of specialty carbons and chemicals from fuels, examination of the degradation of pollutants in the environment, and the combustion of fuels in furnaces and internal combustion engines. Facilities and expertise are also available for the synthesis, characterization, and application of catalytic materials for fuels processing, emissions control, and pollution prevention.

FACULTY

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Philip L. Walker, Jr., Evan Pugh Professor Emeritus of Materials Science, Ph.D. (Penn State)

DR. ALAN W. SCARONI, IN CHARGE OF GRADUATE OPTION

Conclusions (Pyro-Pang ball shaped spheres) generated by rapidly...
The Metals Science and Engineering specialty is science-oriented with a broad range of course work and research in the processing of metals, microstructural evolution, and both mechanical and physical properties. Of special note are strong efforts in corrosion, electrochemistry and aqueous processing, oxidation studies, and laser processing. Research programs in powder metallurgy, deformation and fracture of advanced materials such as intermetallic alloys and metail matrix composites, and phase transformations studies also are extensive.

**FACULTY**

- William R. Bider, Professor Emeritus of Metallurgy, B.S., M.S., Ph.D. (Carnegie Tech)
- Tarunakar DebRoy, Professor of Materials Science and Engineering, B.E. (Burdwan), Ph.D. (Indian Inst. of Science)
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- Earle Ryka, Associate Professor of Metallurgy, B.S. (MIT), Ph.D. (Iowa State)
- George Siukovich, Professor Emeritus of Metallurgy, B.S., M.S., Ph.D. (Penn State)
Polymer science at Penn State is a multidisciplinary subject concerned with the study of macromolecules. Such molecules are pervasive in today's technological society and find numerous applications in such diverse fields as plastics, elastomers, adhesives, surface coatings, textiles, packaging, and composites. Students work with faculty on a wide range of research projects, some of which are outlined in these pages. In addition, special facilities exist for research in the areas of polymer synthesis, polymer blends, surface science, mechanical properties, modeling and theoretical studies, diffraction and scattering, multicomponent systems, polymer characterization, high-temperature stable polymers, conducting polymers, microscopy, vibrational spectroscopy, and thermal analysis.

FACULTY

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Tze-Chiang Chang, Professor of Polymer Science, B.S. (Chung Yuan, Taiwan), Ph.D. (Pennsylvania)

Ralph Colby, Associate Professor of Polymer Science, B.S. (Cornell), Ph.D. (Northwestern)

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Sanar Kumar, Associate Professor of Polymer Science, B.S. (Indian Inst Tech), M.S., Sc.D. (MIT)

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James P. Ruot, Professor of Polymer Science, B.S., Ph.D. (Penn State)
While there is no graduate option specifically in electronic and photonic materials, materials science and engineering faculty are very active in the field, and many electronic and photonic materials projects are available to graduate students. Research in this area at Penn State focuses on diamond, ferroelectrics, gallium nitride, glasses, optical waveguides, silicides, silicon, silicon carbide, and superconductors, as well as some electronic and photonic materials. Special facilities exist for integrated circuit processing, molecular beam epitaxy, pulsed laser deposition, sputtering, spectroscopic ellipsometry, and transmission electron microscopy.

Students interested in electronic and photonic materials may apply to any of the programs within the Department of Materials Science and Engineering (Ceramic Science and Engineering, Fuel Science and Engineering, Metals Science and Engineering, and Polymer Science and Engineering), or the Intercollege Graduate Program in Materials.

FACULTY
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André L. Boehman

Heat and Mass Transfer in Combustion and Pollution Control Systems

Key words: pollution control, heterogeneous catalysts, combustion, heat and mass transfer, organic pollutants, catalysis.

References:


Figure 1: Scanning electron microscope images of diesel particulate matter from (a) a single-cylinder diesel engine and (b) the same engine with catalytic coating applied to the piston crown, cylinder head, and valve. The thrust bearing coating enhances the oxidation of combustible hydrocarbons that originate with the diesel fuel. In Figure 1(b) the particulate matter has a more granular appearance, showing that the soot particles are not bound together by heavy hydrocarbons.

Figure 3: Scanning electron microscope images of diesel particulate matter from a single-cylinder diesel engine and (a) the same engine with catalytic coating applied to the piston crown, cylinder head, and valve. The thrust bearing coating enhances the oxidation of combustible hydrocarbons that originate with the diesel fuel. In Figure 1(b) the particulate matter has a more granular appearance, showing that the soot particles are not bound together by heavy hydrocarbons.

Figure 1: Allyl chains spaced in monolayer on a Au(111) surface.
Paul W. Brown
Chemical Formation of Ceramics and Composites

Contrast to the conventional sintering process for inorganic ceramics at temperatures in excess of 1,800°C, advanced ceramics and novel composites can be formed at low temperature and low pressure through controlled chemical reactions. This method of property enhancement has broad applicability to the fabrication of both monolithic materials and unique-composite materials. Unlike sol-gel recipes, chemical reactions produce near-net shape parts quickly and cost-effectively. The high-temperature process is not required in the shape, as well as low temperature and pressure, involves minimal expansion or contraction. Composites can be made using combinations of materials that would be precluded if they were to occur at high temperature. For example, ceramic-ceramic composites combining nonmetallic constituents such as metals or polymers, can now be formed.

As a general example of a chemical reaction, the formation of a ceramic can be used to illustrate some features of these reactions. For practical application, high toughness can be obtained; for electronic applications, useful properties such as electrical conductivity can be conferred on electronic devices to produce piezoelectric, optoelectronic, or chemostructural ceramics. Dr. Brown's group has demonstrated the mical formations of a variety of ceramics and metallic composites that are formed by the formation of new phases. This work has been synthesized within a few hours at low temperatures and under conditions compatible with those in vivo. Pure phase, porous monoliths of high-sensitivity ceramics have been synthesized easily at low temperatures. These low-temperature processes have been prepared at 0°C, monoliths require the use of high-sensitivity ceramics. This lower-class of ceramics is primarily multifunctional and is of interest as a fast state electrolyte, low thermal expansion, low thermal conductivity material.

Altaf H. Carim
Microstructure at Solid-State Interfaces

Professor Carim's research interests are centered around the microstructure and microchemistry of solid state materials and their interfaces. The primary research tool in this work is the transmission electron microscopy (TEM). Current studies include the exploration of segregation and precipitation at ceramic grain boundaries, development of electron holography, analysis of metal-organic framework (MOF) chemistry, and new composites. Novel composites are formed by novel complex compounds that are often found as reaction products between ceramic and metallic alloys. The structure of interface structures is defective in thin films. The first two processes are briefly described here.

The controlled development of anisotropic microstructures in ceramics holds considerable promise since planar or needle-shaped grains promote crack deflection and lead to a toughening of the material. The relative orientation of the grains and the presence or absence of intergranular precipitates, amorphous layers, and impurity segregation are critically important.

High-resolution transmission electron microscopy (HRTEM) allows us to observe such features on the atomic scale in a sufficiently thin sample. An example is shown in Figure 1.

In this case, the long, flat face of an alumina plate (grain at upper left) exhibits an intergranular amorphous phase at the boundary with an adjacent, randomly oriented aluminum grain. The crystal lattice planes are imaged directly in both grains. In situ chemical analyses by energy-dispersive spectroscopy (EDS) allow us to discern the phases present in each of the wide regions containing the intergranular amorphous phase. Other grain boundaries are devoid of this phase, and no preferential formations along the basal planes of aluminum appears to be closely linked to the development of the anisotropic microstructure.

In this work, the technique of electron holography is being developed and applied to materials problems such as the shape analysis of fine particles. Interferograms are formed by combining a reference electron wave with the wavefunction passing through the sample, as shown in Figure 2. The interference fringes are displaced due to phase changes as the object wave passes through the sample. From the interferograms, the density distribution and the amplitude distribution of the electron wave can be separated, providing a wealth of information on the size, shape, and chemical variations of the object.

Keywords: chemical formation of ceramics and composites; bioceramics, bio-composites, multi-component phase equilibria, low-temperature synthesis

Publications

Figure 1. Transmission electron microscopy (TEM) of a ceramic. The large grains (left) are identified as a needle-like phase. The small grain (right) is an amorphous phase. The large grains exhibit a lattice fringe pattern and the small grains do not. The image was taken at a magnification of 100,000x.

Keywords: transmission electron microscopy, electron holography, microstructure, grain boundaries, intergranular regions, thin films, chemical variations, the interface.
T.C.(Mike) Chung  
New Polymer Chemistry and Materials

Professor Chung is interested in the development of new polymer chemistry that can lead to new materials. One of his current research projects is the functionalization of polystyrene via borane transition and transition metal catalysis. It is known that the incorporation of functional groups to polystyrene is a useful method for modifying the chemical and physical properties of polymers (e.g., adhesiveness, compatibility, and durability). However, functional groups containing polystyrene are very difficult to prepare using transition metal catalysts such as Ziegler-Natta and Metathesis because of catalyst poisoning and other side reactions. Chung’s study investigates a new approach to preparing functional groups by using the reactivity of borane transition and polymers. Borane nitriles have been found to be stable to a wide range of transition metal catalysis during polymerizations. In turn, the borane polymers are easily converted to various functional groups under mild to neutral conditions. A broad range of polystyrenes, such as PS and PP, with various functional groups (e.g., OH, NH₂, and halides), have been prepared.

The borane-containing polymers have also been used as the building blocks for the development of block and graft copolymers. The borane groups can be easily converted to free radical initiators for the graft-from (free radical) polymerizations. Under some reaction conditions, the oxidation of borane groups is selective and graft efficiency is close to quantitative. This chemistry covers a broad range of copolymer compositions, including both hydrophilic and hydrophobic polymeric segments. Several interesting graft polymers consisted of polyisoprene, poly(4-vinyl pyridine), poly(4-vinyl pyridine) and polyisobutylene as the backbone, and several free radical polymers, such as PMMA, PVA, and PAM, have been obtained as the side chains.

Several applications of the resulting new polymers have also been investigated in our laboratory, such as the immobilized catalyst using functionalized polystyrene as the support materials. The catalyst can be recovered and reused for many reaction cycles. The functionalized and graft polystyrene copolymers are very effective for attaching materials to improve the compatibility in polystyrene coating, blends, and composites. By using these copolymers, several new high-impact plastics and composites have been prepared. We are also extending the borane-containing copolymers to prepare boron-containing carbon fiber which could have oxidative stability at high temperature.

Keywords: functional polystyrene, borane polymer, block graft copolymer, immobilized catalyst, boron-containing carbon, boron-containing graphite
Ralph H. Colby

Polymer Dynamics, Rheology of Polymer Melts, Blends, Solutions, Gels, and Other Complex Fluids

Keywords
- polymer physics, rheology, viscoelasticity, structured fluids, complex fluids, scaling models

Professor Coleman is interested in the application of vibrational (infrared and Raman) spectroscopy to the study of multicomponent polymer systems. In favorable cases, the fraction of groups that are directly involved in specific intermolecular interactions (usually hydrogen bonds) can be measured. From these data the equilibrium constants can be obtained that describe the self-association in pure component (colloids) and the interassociation between two polymers of a binary blend. With this information it is not a long step to a description of the thermodynamics of polymer blends that involve strong specific interactions. An expression for the free energy of mixing of such systems has been developed using an association model, and Coleman’s group has been successful in predicting phase diagrams, miscibility windows, and maps for a wide variety of polymer blends. Extension to more complex systems such as ternary blends and copolymer containing multiple specific interaction sites are currently being studied.

Another research area of interest to Coleman involves the search for additives that retard the formation of carbonaceous solids in jet fuels at temperatures exceeding 400°C. In order that adiabatic jet fuels are anticipated to be much more stringent in the next century, when advanced aircraft are expected to fly at speeds exceeding Mach 4. In addition to the complex chemistry of cracking and reforming reactions that occur when jet fuels are subjected to thermal stresses at temperatures above 400°C, carbonaceous solids at these temperatures are being studied using vibrational and NMR spectroscopy. Using these results as a guide, a number of additives have been identified, most notably hexyl alcohol and 1,4-bromoperbenzoate, that retard the formation of carbonaceous solids in Jet A-1 fuels at 425°C.

Figure 1. FTR spectra of STVP-EMA 74/26 blends

Keywords
- polymer blends, phase behavior, polymer vibrational spectroscopy, hydrogen bonding in polymeric materials, jet fuel stabilization
Semih Eser

Carbontization, Mesoporous Development, Carbon Deposition, Activated Carbon Preparation, Hydroprocessing of Petroleum Residua

Dr. Semih Eser is carrying out research on carbonization of petroleum feedstocks, microstructural characterization of solid carbons by digital image analysis, solid carbon deposition on metal and carbon surfaces, thermal degradation of hydrocarbons under supercritical conditions, hydroprocessing of petroleum residua in supercritical fluids, and activated carbon preparation from lignocellulosic materials and coals.

Delayed coking of FCC slurry ovens produces a premium petroleum coke, called needle coke. Needle coke is used in the manufacture of graphite electrodes for use in electric arc furnaces to produce steel and from scrap materials. The most significant property that takes place during carbontization in a delayed coker is the formation of a carbonaceous material. Figure 1 shows a polarized-light micrograph of a carbonaceous material from a slurry-oil sample, indicating the reduction of mesophase spheres that contribute to form anisotropic solid carbon structures. A high degree of anisotropy is found in needle coke, as it is required to manufacture high-performance graphite electrodes.

A major focus of Dr. Eser’s research program is on seeking a correlation between the molecular composition of the slurry oils and the quality of the resulting coals. Digital image analysis techniques developed in his doctoral research program at Koc University, Istanbul, are used to quantify the optical texture of petroleum coals as a measure of coal quality. A combination of gas chromatography/mass spectrometry (GC/MS), solid-state NMR, and Raman spectroscopy are used to characterize the coal matrix. High-performance liquid chromatography can be used to analyze the coal matrix. The research team is developing a comprehensive method for the characterization of petroleum coals from commercial plants.

Hydrogenation of petroleum-coke residua is important for upgrading these materials to produce more gasoline and other valuable distillate fuels.

Dr. K. Gergen’s work on one-step pyrolysis activation to prepare activated carbons from lignocellulosic materials and coals is continued by Ms. Mine G. Unlu for her master’s thesis work. The one-step pyrolysis activation method offers important advantages over the conventional two-step technique with separate carbonization and activation steps.

Publications


Tarasankar DebRoy

Materials Processing and Rate Phenomena

Pallbearers


Keywords: plasma processing, welding, laser processing, thin films, numerical calculation of heat transfer and fluid flow, rare phenomena.

Publications


Figure 1. Polarized-light micrograph of a solid produced by carbontization of a coal oil, indicating the mesophase spheres and their coherence in form anisotropic structures.

Keywords: carbontization, mesoporous, activated carbon, carbon deposition, hydroprocessing of petroleum residua.
The essence of materials science is structureproperty-processing relationships. How do you predict process materials so they have the necessary structure to produce required properties? Polymers are the most widely used class of polymers and include polyethylene (PE) and polypropylene (PP). These two polymers make up more than half of all commercially used polymers. They are among the lowest-cost materials, and yet are some of the most versatile. Modern changes in chemical structure and processing process materials properties as diverse as foamed cushions, bulletproof fabrics, garage bags, insulated cables, food wrap, and medical devices. Dr. Harrison’s work has centered on understanding and developing PE-based polymers.

For any polymer, there is a range of properties that it can have. The inherent range of properties is determined by the polymer’s molecular structure. However, these properties are often not realized unless special processing methods are employed. One method being examined by Dr. Harrison is blending the polymer with other materials. Examples of Harrison’s research in structure six times and polymer blending are outlined below.

Many polymers are made by copolymerization of two or more monomers to produce a polyethylene copolymer. Molecules that make up the copolymer don’t all have the same composition. Although the copolymer has some average composition, a composition distribution exists. The distribution and composition are determined in part by the composition and composition of the PE changes. Copolymer composition changes the way in which the resulting molecules crystallize. This composition allows us to determine composition distribution. The technique, termed TREF (temperature rising fractionation), has been developed at Penn State to a commercial level, and it is operational continues.

Mixing PE with other polymers often produces materials with poor properties. PE, like many other polymers, doesn’t bond to metals. It is incompatible. However, even extremely incompatible materials can be processed to take advantage of unique molecular properties. For example, PE and liquid crystalline polymers (LCPs) can be processed to yield in situ fiber-reinforced materials. With only 10 percent LCP, this copolymer’s stiffness can be made to be five times that of PE. And with additional treatment, it is possible to increase the stiffness of the PE. Since, in general, properties are being evaluated for a number of applications, and further work is designed to take advantage of property combinations in this new class of materials.

The two examples of research given above are not unique. Particularly PE copolymers, as determined by TREF, are easier to process into LCP fiber-reinforced materials. This synergism between copolymers enhances the ultimate utility of these materials.

Keywords: structure-property-processing relationships in engineering, rheology, mechanical properties, elongational behavior, polymer processing and characterization, polymer science, polymer engineering, molecular structures, biocompatible materials, structural behavior, mechanical behavior, brittle materials, failure analysis, micromechanics, fracture mechanics, structural reliability.

Pulitzer


Polymers


Danty J. Green

Professor of Ceramic Science and Engineering

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Keywords: mechanical behavior, brittle materials, failure analysis, micromechanics, fracture mechanics, structural reliability.
spectroscopy to the study of environmental problems, ather research areas involving the use of equipments housed in the Hatch laboratories include nuclear magnetic resonance imaging of coal to examine dimensionally related changes during coal swelling. 13C NMR of coal and microporous solids to ascertain average pore dimensions and pore morphology, and 19F NMR of coal and natural biopolymers, and kinetic studies of the thermal degradation of petroleum and coal-based fuels.

**References**


**Keywords**

environmental chemistry and geochemistry, coal derived biopolymers, lignin, coal, NMR

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**John R. Hellmann**

**Development of Materials with Tailored Properties**

Professor Hellmann’s research interests focus on the development of fundamental principles and materials design methodologies for their application as structural and thermal members in various external applications. These research efforts cover the range from monolithic to composite ceramic and intermetallic materials. Efforts in microstructure control and processing, fracture mechanics, mechanical, electrical, and optical properties of materials are of central interest to his research.

Several studies in Professor Hellmann’s laboratory address tailoring of interfacial bonds in model ceramic/fiber-reinforced compositesendless fibers and intermetallic matrix composites to elucidate the key mechanisms that contribute to enhanced high-temperature fracture toughness and strength of these materials. This research takes a multidisciplinary approach to the development of novel fabrication methods for such materials and opens up a myriad of problems for producing advanced ceramic-composite materials as high-temperature structural components for the aerospace, petrochemical, and automobile-manufacturing industries. Current efforts are concentrated on the development and application of fiber coatings to achieve the levels of interfacial bonding and thermomechanical stress relief required for high fracture toughness and high-temperature strength.

A parallel activity in Professor Hellmann’s laboratory focuses on establishing processing and analysis methods for predicting, and experimentally verifying, physical properties such as thermal conductivity, thermal expansion, heat capacity, optical emittance, elastic moduli, and interlaminar strength of ceramic composite materials with tailored microstructural characteristics. His research team has combined finite-element methods with experimental verification of interfacial shear behavior to assess the relative contributions of thermomechanical stresses and interfacial adhesion to the interfacial failure in fiber-reinforced composites. Results of these efforts have been instrumental in identifying mechanisms contributing to interfacial failure, as well as in establishing criteria for properly quantifying the contribution of each to the overall interfacial failure process. Much effort has been devoted to his laboratory to developing new methods for improving the thermal performance of these important materials to stresses as high as 1500°C in controlled environments. Data compiled in Hellmann’s lab on the temperature-dependent properties of some materials has been employed in prediction of the thermal performance and mechanical reliability of large ceramic components in industrial systems. Field evaluation of full-scale components has lead to applied research and analysis methodologies developed. As more materials and processing improvements are installed in the lab, the research is a success in the lab. Improvements in materials and component designs with confidence in advanced materials for high-temperature industrial, aerospace, and automotive applications.

**Publications**


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**Keywords**

ceramics, intermetallics, composites, interfaces, coatings, mechanical properties, thermal proper ties, processing, microstructure, structure-properties relationships

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**Keywords**

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Donald A. Koss

Ductile Fracture and Failure Criteria of Steels

The performance of load-bearing structures under complex loading conditions obviously depends on the material's mechanical response. Predicting an anticipated performance level of such structures relies on accurate modeling and simulation, which in turn relies on realistic descriptions of the materials' responses under the imposed loading conditions. Such predictions are complicated by the fact that most engineers are typically subjected to multi-axial stress states that are spatially nonuniform and often contain weldments, resulting in material properties that, in turn, vary spatially.

Using Varey HY and HSLA steels as model systems, Dr. Koss's research program examines the multi-axial fracture criterion and fatigue fracture mechanisms characteristic of real base plate and weldments. Based on a combination of experiments and computational analysis, the research has two primary goals. The first goal is to determine the failure strains of steel weldments as a function of multiaxial stress states and in a form that can be implemented into existing failure codes. The second, more fundamental goal is to establish the mechanisms of failure and their sensitivity to stress state, and to incorporate this information into existing failure models in order to improve their accuracy. The program consists of several components: an experimental study to determine failure conditions and the underlying fracture mechanisms, a computational modeling study to address the "void-shear" mechanism of ductile fracture, and an experimental modeling effort to identify void interactions during fracture.

Publications

Figure 1. A failure limit diagram indicating failure stress as a function of multiaxial strains for HY-100 steel.
Thermodynamics of Complex Condensed Phase Systems, Polymers at Surfaces and Interfaces, Glass Transition Phenomena, Dynamics of Macromolecular Liquids

Digby D. Macdonald
Improved Control Over the Operation of Thermal Power Plants

Dr. Digby D. Macdonald is the director of the Combustion Advanced Materials and a professor of materials science and engineering at Penn State. He holds B.Sc. and M.Sc. degrees from The University of Auckland, New Zealand, and a Ph.D. from The University of Calgary, Alberta, Canada.

A native of New Zealand, Dr. Macdonald became an U.S. citizen in 1984. Prior to joining Penn State in 1991, he was the director of the chemistry laboratory (1984–87) and the materials laboratory (1987–91) at SRI International (formerly the Stanford Research Institute) in Menlo Park, California. During this latter period, he also served as deputy division director of the physical sciences division of SRI. From 1979 to 1984, he served as a professor of metallurgical research and director of the Furnace Corrosion Center at The Ohio State University.

Since 1993, Professor Macdonald has been a member of the United States Air Force Scientific Advisory Board (SAB) and a member of the SAB Materials Panel, recently led a study under the auspices of the National Institute of Standard Technology to explore and define the future materials needs of the air force. Dr. Macdonald received the Whitney Award from NACE-International (1993) and the Wager Award from the Electrochemical Society (1993) and was chosen by the Atomic Energy of Canada, Ltd. to deliver the 1993 W. B. Lewis Lecture in recognition of his contributions to the development of nuclear power in the service of mankind. He is a fellow of NACE-International, the Electrochemical Society, and NACE-International and the Electrochemical Society. Dr. Macdonald is the author of one hundred papers and more than 400 papers in thermodynamics, electrochemistry, corrosion science, chemistry, and material science. He was recently elected to the Royal Society of Canada. Two of Professor Macdonald’s principal research areas are (1) defining the mechanisms of the growth and breakdown of passive films on reactive metal surfaces in contact with aqueous environments, and (2) the prediction of corrosion damage. Within the field of metallic corrosion, he has been instrumental in developing the potent defect model for the growth and breakdown of passive films, which provides a deterministic account of the formation and disruption of passivity on reactive metals and hence the nucleation of localized corrosion damage. He has extended this work to develop “defect functionality analysis” (DFA), which seeks to provide a deterministic basis for predicting corrosion damage in complex systems. For this development and application of this science to nuclear power reactors, and the rejection of the electrochemistry of reactive heat transport circuits, that he was selected as the W.B. Lewis Award in 1993. He is currently developing DFA as a replacement for the empirically based damage analysis techniques that are currently used in nuclear power reactors.

Publications

Keywords
- thermodynamics, electrochemistry, corrosion, high-temperature aqueous systems, stress corrosion cracking

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Figure 1: An optical micrograph of phases separated polymer matrix.

Keywords
- polymers, surfaces, thermodynamics, statistical mechanics, neutron scattering and reflectivity, dynamics, glass transition

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Keywords
- electrochemistry, corrosion, high-temperature aqueous systems, stress corrosion cracking

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Gary L. Messing
Ceramic and Particulate Materials Processing

The fabrication of advanced ceramics with targeted properties requires careful control over all process steps from powder synthesis through sintering. The complex relations between the myriad processes involved in ceramic processing is the general focus of Dr. Messing's research program. For example, he and his group have had a marked effort to understand how to regulate ceramic phase development through the application of fundamental concepts of epitaxy. By using seed crystals, or by developing self-nucleating sol-gel chemistry, they have demonstrated unique control of phase development, transformation kinetics, sintering, and microstructure development in alumina, alumina-based ceramics, and mullite. Recent progress in template grain growth has resulted in single crystals and highly textured ceramics. Spray pyrolysis is a unique process for the synthesis of advanced powders and films from solution droplets. Messing's group has a comprehensive research program designed to identify how each of the processes during spray pyrolysis can be regulated to yield particles of controlled size, morphology, and chemistry. They are also developing experimental methods and in situ diagnostics for the on-line monitoring and investigation of the individual processes responsible for particle formation. By regulating the thermodynamics of the particulate materials and films of mixed metal oxides, nanocrystalline composites, and metals can be prepared.

Figure 1. Schematic of spray pyrolysis system.

Keywords
Ceramic processing, powder synthesis, spray pyrolysis, solid-phase epitaxy and phase transformations, sol-gel, sintering
Robert E. Newnham is Alumni Professor of Solid State Science and associate director of the Materials Research Laboratory. Recently elected to the National Academy of Engineering, Newnham has written nearly 300 research papers on electronic ceramics and microelectronics. During the past two years, he has been awarded the Ceramic Prize by the Ceramic Society of Japan, the John E. Hopwood Medal of the American Ceramic Society, the Turnbull Prize of the Mineralogical Research Society, and the British Ceramics Institute Prize of the Academy of Ceramics for his "outstanding and creative contributions to the advancement of ceramic science and art, especially in the field of microstructural ceramics research. Newnham is active in several professional organizations, having served as editor of the Journal of the American Ceramic Society, President of the American Ceramic Society, Association, and Distinguished Lecturer for the Institute of Electrical and Electronic Engineering.

The current research program is centered on "smart" and "very smart" ceramics. Smart ceramics are defined with respect to the sensing and actuating functions of living systems. A smart ceramic senses a change in the environment, and a feedback system makes a useful response. It is both a sensor and an actuator. Applications include vibrational damping, space systems, and energy-saving windows for homes and facilities. The new electronically controlled automobile suspension systems made from multilayer piezoelectric sensors and actuators are also classified as actively smart materials. By building in a learning function, the definition can be extended to a higher level of intelligence: a very smart ceramic senses a change in its surroundings and responds by changing one or more of its properties. Such a material can tune its sensing and actuating functions in time and space to optimize behavior. The distinction between smart and very smart materials is essentially one between linear and nonlinear properties. The physical properties of nonlinear materials can be adjusted by bias fields or forced to control response.

Newnham is currently developing a family of tunable transducers, which utilize the nonlinear properties of relaxor ferroelectrics interfaced with thin layers of rubber and metal components. The basic design is patterned after metal-ferroelectric composite actuators developed in his laboratory (Figure 1). Shallow cavities positioned between the metal caps and the central ceramic disk convert and amplify the radial displacements of the piezoelectric ceramic into the large axial motions of the metal end caps (Figure 2).

Five important characteristics of an electromechanical transducer are the resonant frequency, the electromechanical coupling coefficient k, the acoustic transduction Zp, and the electrical transduction Zl. In the tunable transducer, the magnitudes of k, Zp, and Zl are controlled by stretching thin layers of rubber, while k and Zl are manipulated by applying bias fields to the outer layers of relaxor ferroelectric such as magnetostrictive PMN (27). As shown in Figure 3, electromechanical PMN gives larger strains than the usual ZT transducers.

The search continues for "smarter" ceramics for use as sensors and actuators. The nonlinear properties of very smart materials are often associated with nanoscale structures and diffuse phase transformations. Under these circumstances the structure is poised on the verge of an instability, and responds readily to the influences such as electric or magnetic fields, or mechanical stress.
Research on particle design needs to create environments that systematically constrain particle morphology, growth, and aggregation. In the gel-sol method, highly condensed natural hydroxide gels are used as the matrix for the growth of metal oxide particles. The viscous environment restricts particle movement and thus particle aggregation is minimized. Under investigation is microemulsion-mediated synthesis where surface-stabilized nanoscale emulsions constrain the growth of nanoparticles. Emphasis is on the relationships between the properties of the microemulsion fluid phase and particle characteristics.

Important engineering applications of dissolution processes are encountered in hydrometallurgical extraction, surface finishing, and semiconductor device technology. Research in progress focuses on the electrochemical behavior of metallic, semiconductor, and insulator materials. Of particular interest are the rheo-electrochemical models of the solvent solid-solution equilibria and the reduction of the solute-induced defects, surface completion, and semiconductor electrochemistry.

Interfacial phenomena underlie many of the techniques available for ion and particle separations. Surface-solution phenomena are under investigation in connection with reversed micelle catalysis of hydrometallurgical liquid-solid extraction. Polymer-solvent interactions can induce phase separations in aqueous systems. Particulate separations that use such aqueous phases as liquid-liquid transfer media are being developed.

Paul Painter

Paul Painter is interested in the effect of strong specific intermolecular interactions on the properties of polymers, particularly their ability to mix with solvents, other polymers, and liquid crystalline materials.

In describing the mixing of non-electrolytes, it has been common to distinguish between so-called "normal" and "associated" liquids. The most common examples of the latter type correspond to molecules such as water, alcohols, amines, etc., that form hydrogen bonds. At an early stage, the assumptions of simple models, such as regular solution theory, were recognized as too crude when applied to these types of mixtures, and their unusual or anomalous properties could only be accounted for by recognizing that the molecules were associated in a specific manner. Indeed, many years ago, Prigogine proposed that the formation of a complex be treated by using the assumptions of a chemical equilibrium between the hydroxyproton of the associated species, and this approach has been the basis for the use of so-called association models.

Association models have, until recently, been largely ignored in treating hydrogen bonding in polymer mixtures. They have most frequently been applied to mixtures of alcohols with simple hydrocarbons, where the equilibrium constants used to describe association have usually been determined by a fit to thermodynamic data (e.g., vapor pressures, heating of mixing). In collaboration with Dr. Michael Coleman, Painter has sought to do two things: first, to adapt this approach to a description of the phase behavior of polymer mixtures; and second, to develop spectroscopic methods that provide an independent measurement of the equilibrium constants. A model has been developed that provides a good description of the phase behavior of these types of mixtures.

Keywords
aqueous processing, particle design, materials synthesis and processing, hydrometallurgy, separation science, wet processing in semiconductor technology, surfactants, colloids, interfaces

Figure 1. High pressure hydrogen bonding in poly (vinyl alcohol).

Effects of Strong Intermolecular Interactions on the Properties of Polymers

Publications

Keywords
Hydrogen bonding in macromolecular systems (polystyrene and coals, polymer blends, gels, liquid crystal/polymer mixtures, coal structure)
Coal is one of our major energy sources today and will continue to be in the near future. The use of coal as a fuel has negative effects on the environment in terms of pollution. With an increasing concern for the environment, coal combustion technologies are needed so that we can keep using coal for power generation. Fluidized-bed combustion is such a technology, with low emissions of nitrogen oxides (NOx) and sulfur oxides (SOx)—the main pollutants from coal combustion. A side effect of fluidized-bed combustion is the formation of nitrogen oxide (NOx). Unlike NOx and SOx, nitrogen oxide is not widely known as a pollutant, but it has been identified as a greenhouse gas and plays a role in the depletion of the ozone layer. The research interests of Professor Pers are centered around developing clean coal technology that incorporates NOx and SOx reduction strategies. His focus is on radiation-induced NOx and SOx emission control and catalytic gasification of coal.

Radiation-induced removal of NOx and SOx from flue gases is an emerging technology, with a high potential of becoming a competitive alternative to more traditional NOx and SOx reduction techniques. One of its strengths is that both pollutants can be efficiently eliminated in a single unit operation. The principle of this technology is that a blue gas is subjected to fast electrons. These electrons can be generated in different ways. One possibility is to use electron guns (so-called e-beams) that accelerate electrons and shoot them into the flue gas. Another option is to let the flue gas pass through a strong electromagnetic field in which a non-thermal plasma is generated. In both cases, fast electrons initiate a series of radical reactions that result in the reduction of NOx and SOx to nitric and sulfuric acid. By the addition of ammonium salts, which are formed during the process of the gas, calcium can be removed from the gas using electronic precipitators or bag house filters. As just as ash is removed, the challenge is to manipulate the reaction conditions in such a way that nitrogen oxide emissions are diminished without sacrificing the reductions in NOx and SOx emissions already accomplished. Coal gasification is one way to combine the chemical cycle that is implemented in a new generation of coal-fired power plants. By gasification of coal, a combustible coal gas is produced that is used later in the process for combustion. It is much easier to remove nitrogen and sulfur compounds from coal-derived gas than from flue gases. The addition of catalysts can enhance the performance of the gasification, e.g., lower temperatures at which gasification can be carried out, or higher reaction rates at the same temperature. Catalysts also influence the composition of the coal-derived gas, and careful selection of a catalyst is necessary.
Howard W. Pickering  
Corrosion and Electrodeposition of Metals

Sarma V. Puspati  
Emissions Control from Stationary Combustion Systems

Keywords: surface properties, electrode reactions, corrosion of metals, electrodeposition, scanning probe microscopy.

Dr. Puspati's research interests are primarily in the experimental study of carbon-based combustion models, including coal combustion and pulverized coal combustion. Specific research topics include: coal-water slurry combustion; combustion behavior of coal; and the effects of biomass-based fuels. The research focuses on the development of advanced emission control technologies for stationary combustion systems.

Sarma V. Puspati  
Emissions Control from Stationary Combustion Systems

Keywords: fluidized bed combustion, SO2 capture, biomass, simultaneous SO2 and NOx reduction, biofuels.
Professor Randall's research interests are in processing and microstructural-property relations in advanced ceramic materials. Special attention is given to the problems incurred in the optimization and tailoring of dielectric properties as so to address issues such as device miniaturization and component integration for low loss and high performance.

With recent advances in the fabrication of ceramic particulate materials, there exists a need to improve processing assembly techniques to control novel architectures at finer scales. We are investigating the use of electric fields to assemble particulates in composite and thin film devices. In general, when an electric field is applied the stable suspension, the particle motion is predominantly dictated by dielectrophoretic and electrophoretic forces. Dielectrophoretic assembly involves the induction of a dipole-dipole interaction through dielectrophoresis in such a way that the particles undergo unidirectional aggregation along the electric field direction. This process has been studied in thermotropic polynematics that undergo a nematic-uniaxial transition to produce uniaxial composites with dielectric anisotropy.

Electrophoretic deposition exploits an electric surface charge on particles in suspension migrating in the presence of an appropriate electric field enabling the consolidation of particulate matter into desired structures. By understanding the colloidal stability, the deposition kinetics, and the constrained drying issues permitted fabrication of 10-50 micrometers BaTiO3 thin films with high dielectric constant and low losses comparable with other thin film deposition technologies. The ongoing work is focused on establishing the scientific and engineering aspects of the deposition process. Electrophoretic deposition of dielectric ceramic particulate materials give potential advances in a number of applications, including pyrotechnics, biomedical ultrasound probes, and heterogeneous chemical sensors.

Ferroelectric and related materials are of interest due to their unique elastolectric properties being used in piezoelectric, electrostrictive, pyroelectric, and capacitive applications. Our group has focused attention on the role of microscopic situations on physical properties. Recent work using detailed transmission electron microscopy studies (in-situ and ex-situ) have been the grain size effects on domain switching mechanisms during poling and de-polar-induced spatial modulations with deformations in which show a strong influence on the dielectric property contributions to physical properties. With grain sizes below 1 micron, a change in the domain structure and reduction in the number of domain variants per grain, has resulted in there is a reduction in the dielectric and piezoelectric properties. By understanding the
Multicomponent Polymer Systems


Figure 1. Schematic of three possible microstructures of a mixture of lithium binary blend of on one phase ( ) and semi-crystalline ( ) polymer. A: Amorphous polymer is interfacial 1 and 2, B: Amorphous polymer is interfacial 1 and 2.

Jerzy Ruzyllo
Surface Processing in Microelectronic Manufacturing

Professor Ruzyllo is concerned with integrated circuit manufacturing science and engineering, with an emphasis on silicon surface cleaning using gas-phase processes. His research currently stress gas-phase treatments aimed at the removal of chemical contaminants from the silicon surfaces, and also developing techniques for gas-phase surface processing in microelectronics manufacturing. In addition, he is actively involved in the development of methods for in situ, real-time process monitoring in microelectronics manufacturing. He has a continuing interest in the role of carbon in silicon (particularly during thermal oxidation) and is expanding his research in this area to include work on SiC processing for microelectronics applications.

Wafer cleaning is the most frequently applied processing step in the microchip manufacturing sequence. The commonly-used technology of liquid-phase (w) wafer cleaning will remain a dominant cleaning method in this area, however, wafer cleaning technology has a number of inherent shortcomings that may limit its usefulness in fabricating future generations of integrated circuits. Consequently, the need to develop gas-phase (dry) wafer cleaning methods was recognized, and appropriate research was initiated, several years ago. Ruzyllo and his graduate students have participated in this effort since its beginning. They developed the reduced pressure ash borosilicate (AHP/ARH)/alkaline soluble etching of native chemical oxide, as well as the overall dry cleaning procedure involving the operation carried out in sequence without breaking the vacuum: UVO, AHP/ARH mixture, UV/ARC, LCO/ARC. This sequence was successfully implemented as a pre-gate oxidation clean in the gate stack cluster tool. In addition, Ruzyllo led the development of gas-phase method of pass RIE surface processing that includes a UV/ARC polymer removal process and a UV/ARC, “soft etch” of silicon, resulting in damage- and contamination-free surfaces.

Keynotes
- Microelectronics, silicon wafer cleaning, wafer conditioning, in-line process monitoring

Publications


Earle R. Ryba

Determination of the Structures of Quasicrystalline Materials

Quasicrystals are materials whose X-ray and electron-diffraction patterns exhibit non-crystallographic symmetries, such as five-, eight-, and tenfold rotation axes. These fivefold symmetry elements in the diffraction patterns help explain the long-range but noncrystalline order in these materials in which the atom positions form an aperiodic, noncrystallographic, fivefold decagonal order. While this general picture of the connections between the atoms is known, the lack of a three-dimensional periodic repeat unit, or unit cell, has made the determination of the structure of these materials extremely difficult. At Penn State, we have been successfully studying the structure of quasicrystals to determine the existence of these strange materials and to advance our understanding of them.

Recently, our studies have focused on the decagonal phase of Al₇₃Cu₁₇Si₁₀. In this system, the structure of the compound exhibits non-crystallographic symmetry in two ways, which is a crystalline phase in a single crystal. Furthermore, from a considerable number of X-ray and electron diffraction evidence, we have found that its structure is even more complex. Embedded in the quasicrystalline structure are extended regions of periodic atomic arrangement, in which a very large three-dimensional unit cell is formed from several of these regions. In addition, the size and shape of the unit cell are periodically arranged regions of the structure, depending upon composition and cooling conditions.

We have formulated a comprehensive model for the structure of this decagonal phase and crystalline regions using electron and X-ray diffraction and the results of high-resolution electron microscopy and scanning tunneling microscopy. This model is built from four primary atomic clusters that are present in both the Al₇₃Cu₁₇Si₁₀ and Al₇₃Cu₁₇Si₁₀₅ phases. This model is consistent with the recent electron diffraction patterns and X-ray diffraction patterns of the decagonal phase of Al₇₃Cu₁₇Si₁₀ and Al₇₃Cu₁₇Si₁₀₅.

Alan W. Scaroni

Combustion of Fossil Fuels

The impact of fossil fuel combustion on the global environment requires that efficiencies be improved and emissions reduced. This is especially the case for solid fuels such as coal. The environmental performance of existing power systems needs to be improved and new systems designed to meet the environmental performance expectations of the next century. A particular challenge is to design “zero discharge” power plants that incorporate processes that eliminate the emissions of acid gases such as sulfur dioxide and nitrogen oxides, trace elements including heavy metals, and volatile organic compounds.

Professor Scaroni’s group has been working for more than a decade on understanding the processes that produce emissions of pollutants and developing technologies for reducing their emission into the environment. A substantial effort has been in the area of sulfur dioxide capture by limestone in fluidized bed combustion. Before the group’s research revealed the importance of thermodynamically induced phenomena to the efficiency of sulfur capture, limestone was inappropriately specified on the basis of calcium carbonate content. Recent work has shown the importance of grain size in controlling particle size, another important aspect of performance.

Forced oxidation limestone scrubbers are used for post-combustion control of sulfur dioxide in commercial coal-fired power plants. Recent results point to the importance of the dissolution rate of the limestone in the scrubber to the overall performance of the unit. Ongoing work is aimed at understanding the limestone properties that control dissolution rate.

In the area of nitrogen oxide formation and control, the group used “N MEMS” spectroscopy to establish the importance of pyrolysis in the coal structure as a source of nitrogen oxides. Prior to this pioneering work, pyrolysis nitrogen was thought to be the dominant source. With industrial partnerships, low NOX burners have been designed and tested and are now being produced commercially. In addition, the performance of industrial burners has been predicted computationally, and the group has established the importance of flame structure to combustion efficiency and NOX emissions.

Publications


Keywords

Keywords

X-ray diffraction, structure of thin films and interfaces in composites, grain incursion diffraction and X-ray reflectometry, structure of intermetallic compounds, mechanism of sintering in powder metallurgy

Keywords

coal, combustion, fluidized beds, sulfur fuels, combustion-generated pollutants.
Darrell G. Scholm

Molecular Beam Epitaxial Growth of Oxide Thin Films

This research focuses on the mechanism of coal and petroleum derivatives (particularly new approaches for refining) and conversion to other fuel forms, chemical feedstocks, or carbon materials. A major research effort is in the development of coal-based jet fuels. High-performance aerospace aircraft develop significant heat loads from the heat released in the engine. A solution to this problem is to use the aircraft’s jet as a heat sink to cool hydraulic fluids, sensitive electronics, and engine components. The thermal stressing of the fuel in such situations can cause in pyrophoric decomposition, leading to the formation of carbon deposits. If these deposits plug jet fuel lines or burn near nozzles in the engine, a catastrophic could result. The goal of the coal-based jet fuel project is to develop a fuel formulation, combining coal-derived liquids with petroleum refinery streams, that will withstand temperatures of up to 900°F without serious deposition problems.

Coal-based jet fuels are more stable in the high-temperature pyrophoric decomposition regime than current petroleum-only fuels. The key difference is the higher proportion of pyrolysis and pyrohydrogenation components in the coal-based fuels. Because coal has molecular structures mainly on pyrolytic aromatics, the potential exists to produce highly stable jet fuels by chemically removing the pyrolytic aromatic structures from the macro- molecular coal structure and hydrogenating the resulting coal-derived pyrolysis aromatics or pyrohydrogenation.

Other current research projects focus on the use of coal as a feedstock for the production of carbon-based materials, modifying heavy petroleum-derived materials, such as pitches, for production of carbon, and novel approaches to upgrading petroleum residues by direct reaction with methane. Computer modeling of the molecular structures in coal and neural network computing of viscosities of molten coal ashes are also active projects.

Keywords

- oxide film growth, molecular beam epitaxy, pulse laser deposition, high temperature superconductors, ferroelectrics, thin films, MBE, PLD

References

Chunshan Song

Catalysis in Fuel Processing and Shape-Selective Catalysis

Karl E. Spear

High-Temperature Materials Chemistry

Chemical interactions at high temperatures are critical in the synthesis, fabrication, consumption, and environmental disposal of materials. Dr. Spear's research has focused on predicting and understanding the high-temperature behavior of materials through experimental and theoretical applications of high-temperature chemistry principles. Phase equilibria, and thermodynamics. Major areas of research have included nuclear fuel materials, metal oxide binders, and the processes of CVI, oxidation, and corrosion. Interface reactions in composites, thermal analysis of glass systems, and the vapor deposition of diamond. Spear and his colleague Michael Frenklach began developing molecular models for the structural synthesis of diamond using atomic models of diamond (sp3) and single-crystal faces, and the diamond's high temperature stability. The use of such models to predict the behavior of CVI diamond and to determine the role of atomic interactions in diamond growth is illustrated in Figure 1. The diamond deposition process is shown in Figure 2.
Richard E. Tessler

Degradation of Ceramics, Fibers, and Composites

In many energy conversion systems and high-temperature processing plants, abraded ceramics with the requisite thermomechanical properties are thermomechanically unstable in the corrosive environments of the operating system. However, passive reaction products and very slow kinetics may permit adequate lifetimes for many applications. Improvements in materials and protection schemes can best be developed when the processes that cause the corrosion and substitute degradation are understood in detail in terms of rate-limiting reactions and local thermodynamic equilibria.

The long-term reliability of advanced structural ceramics, ceramic fibers, and ceramic-composite materials under static or cyclic stresses at elevated temperatures is dominated by two factors: the first is the importance of mass-stress gradient, the second is the materials characteristics that control these processes, and the third is the need to develop new, reliable, and digenous materials that must be considered for advanced applications. The study of damage mechanisms of commercially available materials must be developed to assure timely application of these materials.

Publications


Susan Troller-McKinstry

Structure-Microstructure-Property Relations in Electroceramic Films

Keywords
ferroelectricity, spectroscopic ellipsometry, thin films, electroceramics

Walter A. Yarbrough

Synthesis and Preparation of Materials

Yarbrough has shown that the relevance thermodynamic model used to determine the solid surface in liquid equilibrium with vapor phase in contact with the solid. These thermodynamic potentials differ from those appropriate for the bulk solid. With this approach, Yarbrough has shown that many diamond-growth methods can be understood since at high atomic hydrogen concentration, the diamond surface formation is more stable than that of graphite. For example, the dominantly observed surface of graphite, the (001) face, is stable on high atomic hydrogen concentration. However, the (111) face is stable on high atomic hydrogen concentration.

The successful use of this formulation as a guide to understanding the growth of diamond implies a useful paradigm in materials synthesis. If accommodation or transformation in the bulk solid can be ignored, as is true with many re-entrant phases, the solid structure can be achieved by adjusting synthetic parameters to control the surface area and the crystalline growth process. Thus, the challenge with cubic boron nitride synthesis may well lie with the question of what conditions stabilize the solid surface to the desired crystal phase by controlling nucleation and growth. Research exploring this and other similar possibilities is continuing.

Professor Yarbrough's major research interest is in understanding the synthesis and preparation of materials. A major focus continues to be the use of microstructural development and phase transformation in the fabrication of materials which are influenced by the presence of surfaces and interfaces. These interests include the nucleation and growth of both single-phase and two-phase materials. He and his students have recently concentrated on the synthesis of metastable phases, particularly diamond and cubic boron nitride, through the use of chemical vapor deposition (CVD). Although early reports from Russia and Japan show that well-crystallized diamond could be synthesized using CVD methods with considerable skepticism, by 1984 it became apparent that the reports were accurate. Much of the early skepticism in the scientific community derived from the well-known phase diagram for solid carbon, which suggests that the formation of diamond from graphite should be impossible at pressures less than approximately 15 GPa. Thus, Yarbrough and his students are focusing on two major issues.

The first of these issues is the question of why well-crystallized diamond can be formed during CVD and not during one of the many other possible carbon phases. What is the critical factor that dictates the structure and crystallographic perfection of the solid diamond formed in CVD? Clearly related to this is the second issue: Can other similar by valuable but metastable crystal phases be synthesized using CVD and related methods? This issue is crucial because it helps to select optimal conditions for novel materials synthesis and fabrication. Parameters among the various materials of interest are the substrate, high, background, gas concentration, temperature, and gas control. For example, in the case of diamond, this means that SE ridges the gap between existing tools designed to characterize the bulk of the solid phase or the surface properties of thin films by spectroscopic ellipsometry. Spectroscopic ellipsometry (SE) is a non-destructive technique capable of depth profiling the dielectric functions of materials with an approx. 0.1 nm resolution over a depth comparable to the penetration depth of light in the material. In the case of diamond, this means that SE bridges the gap between existing tools designed to characterize either the bulk or surface of crystalline materials. Both in situ and ex situ SE are utilized to examine the role of deposition and annealing processes on the homogeneity of thin films. For example, the dependence of Vickers hardness on the oxygen sensitivity of SE is being used to study oxygen diffusivity in diamond thin films. This should enable an improved understanding of the critical factors affecting the properties of superconduction junction devices.
Interdisciplinary Activities

THE MATERIALS RESEARCH INSTITUTE (MRI)

Dr. Rodney A. Erickson
Vice President for Research and Dean of the Graduate School

The Materials Research Institute (MRI) is an umbrella coordinating organization for the large and diverse materials research community at Penn State. The MRI Advisory Board is composed of representatives of the many departments, centers, and laboratories that perform materials research. The board’s objectives are to communicate a coherent picture of research results and capabilities to current and prospective sponsors, to present its collective needs to the University administration, and to coordinate the preparation of major University-wide initiatives and proposals.