P

nen 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 the amount of research support obtained from government and industry.

Graduate study in materials science and engineering is centered at the Penn State University Park Campus. The University Park Campus, the original and largest campus, has almost 32,000 undergraduates, more than 6,000 graduate students, and more than 2,300 faculty, and offers more than 240 degree programs, plus numerous additional options. It is located in the Allegheny Mountains, adjacent to the town of State College in the geographic center of Pennsylvania.

Materials Science and Engineering is one of six departments in the College of Earth and Mineral Sciences. The college has a strong focus on research and graduate education, with programs in materials and mineral engineering and earth sciences.

Faculty in the Department of Materials Science and Engineering also participate in the interdisciplinary Intercollege Graduate Degree in Materials. Many also participate in research projects in the various cross-disciplinary centers such as the Center for Advanced Materials, the Particulate Materials Center, the Energy and Fuels Research Center, the Intercollege Materials Research Laboratory, and the Electronic Materials and Processing Laboratory. Several materials science faculty members have been appointed to the Materials Research Institute Advisory Board, the umbrella coordinating group in materials research at Penn State.

Penn State offers all the facilities of a major university and a full calendar of University lectures and other academic events. The performing arts series brings leading performers from around the world and exciting professional musical, theatrical, and dance productions to campus. A number of other organizations sponsor a wide range of cultural events. The newly renovated Palmer Museum of Art, an important center for the visual arts, hosts a range of exhibitions. The University has truly outstanding recreational facilities and is the site of regularly scheduled sporting events.

The University Libraries has holdings of about 3.3 million volumes with online catalog access. The central library, Pattee Library, is supplemented by specialized libraries, including the College of Earth and Mineral Sciences Library housed in Deike Building.
The Department of Materials Science and Engineering at Penn State, as now 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. As 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 metallography in 1917–1918 and in ceramic technology in 1923. Fuel 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 Intercollege Graduate Program in Materials, completes what is today one of the finest and best-balanced departments of materials science and engineering in the country.

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 Intercollege 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 post-doctoral and graduate students from a wide spectrum of disciplines. There are 40 full-time faculty members, some 200 graduate students, and about 175 undergraduates currently in the department. Materials Science courses that cut across disciplines are offered, in addition to those offered in the specialties. Students are encouraged to broaden their horizons by taking those 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. The faculty have consistently been rated well above average as teachers by students and alumni. Eight of the current faculty have won college-wide teaching awards. Research productivity of the faculty as a whole 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 (in excess of $13 million in outside funding in 1992–93).
General Admission Requirements for the Graduate Program

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 option 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 the department and should be returned to the Graduate School. Application forms for research assistantships should be forwarded to the graduate program coordinator in the Department of Materials Science and Engineering, whose address 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 1993-94 academic year, these paid between $12,680 and $13,600 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 student 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 electromicroscopy, phase equilibria, mechanical properties, thermal properties, surface characterization and properties, high-temperature reaction kinetics, coatings and thin films, solid-state synthesis, dielectric and ferroelectric studies, corrosion studies, and composite materials.

FACULTY

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David J. Green, Professor of Ceramic Science and Engineering: Chair, Ceramic Science and Engineering option, B.Sc. (Liverpool), M.Sc., Ph.D. (McMaster)

John B. Hallam, Assistant Professor of Ceramic Science and Engineering: Associate Director, Center for Advanced Materials, B.S., Ph.D. (Penn State)

Gary E. Menninger, Professor of Ceramic Science and Engineering: Director, Materials Science Center, B.S. (Alfred), M.S., Ph.D. (Florida)

Robert E. Newnham, Alcoa Professor of Solid State Science, B.S. (Harvard), M.S. (Colorado), Ph.D. (Pittsburgh), Ph.D. (Cambridge)

Carn G. Panassio, Professor of Materials Science and Engineering: Director, Materials Characterization Laboratory, B.S. (NJIT), M.E., Ph.D. (Florida)

David E. Panosia, Adjunct Professor of Ceramic Science and Engineering, B.S. (Purdue), Ph.D. (Rensselaer)

Guy E. Rindone, Professor Emeritus of Ceramic Science and Engineering, B.S. (Pitt State)

Karl C. Spurr, Professor of Ceramic Science, B.S. (Baker), Ph.D. (Kanata)

Vladimir S. Stepanian, Professor Emeritus of Materials Science and Engineering, D.Sc., Ph.D. (Zagreb)

Richard E. Trenler, Professor of Materials Science and Engineering: Head, Department of Materials Science and Engineering, B.S. (Pitt State), M.S. (MIT), Ph.D. (Pitt State)

William O. Williamson, Professor Emeritus of Ceramic Science and Engineering, D.Sc. (London)

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Walter A. Yarbrough, Assistant Professor of Ceramic Science and Engineering, B.S. (Univ. NC), Ph.D. (Pitt State)
The Fuel Science specialty at Penn State provides advanced knowledge and research opportunities in the characteristics and use of fuels, including their conversion to other fuels and to other materials. Special facilities exist for research in areas of combustion of fuels, coal ash behavior, coal pyrolysis, catalysis, fluidized-bed combustion, shock-tube studies, coal and carbon characterization, carbonization, coal gasification, and fundamental flame studies.

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Howard B. Palmer, Professor Emeritus of Energy Science, B.S. (Carnegie Tech), Ph.D. (Wisconsin)

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Francis J. Vannala, Professor Emeritus of Fuel Science, Ph.D. (Penn State)

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

Peter M. Walsh, Associate Professor of Fuel Science, B.S. (Rutgers), M.A. (Wesleyan), Ph.D. (Cornell)
Polymer Science (PLMSC)

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, diffusion and scattering, multicomponent systems, polymer characterization, high-temperature stable polymers, conducting polymers, microscopy, vibrational spectroscopy, and thermal analysis.

FACULTY

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Michael M. Coleman, Professor of Polymer Science, B.S. (Borough Polytechnic, London), M.S., Ph.D. (Case Western)

Bernard Gordon III, Associate Professor of Polymer Science, B.S. (Cal Poly), Ph.D. (Arizona)

Ian R. Harrison, Professor of Polymer Science, B.Sc. (Leeds), M.S., Ph.D. (Case Western)

Donald E. Kline, Professor Emeritus of Materials Science, B.S., Ph.D. (Penn State)

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

Paul C. Painter, Professor of Polymer Science, Chair, Polymer Science option, B.S., M.S. (London), Ph.D. (Case Western)

James P. Ranu, Professor of Polymer Science, B.S., Ph.D. (Penn State)

DR. PAUL C. PAINTER, IN CHARGE OF GRADUATE OPTION
**David L. Allara**

**Chemistry at Interfaces**

David L. Allara's research interests involve the study of combustion and pollution control systems for applications ranging from automobile catalytic converters to coal-fired power plants. His research efforts have included the development of experimental facilities designed specifically for the study of pollution control catalysts and numerical models for the dynamic behavior and stress formation within catalytic combustors for natural gas-fired regenerative plants.

Many combustion and pollution control research problems involve the interaction of convective heat and mass transfer and heterogeneous chemistry. Such systems are of tremendous practical importance, and understanding their behavior and finding ways to enhance their performance are essential areas of research.

Within the Fuel Science program, Professor Allara is constructing laboratory facilities for studying pollution control devices and advanced catalysts for use in diverse applications including diesel oxidation and lean NOx catalysts and NOx abatement systems for industrial coal boilers.

Another ongoing research includes the development of a numerical model for the transport of natural gas-fired catalytic combustors. The current form of this computer code is 2-D and includes surface chemistry for an advanced palladium oxide catalyst formulation and thermal stress formation in the ceramic combustor substrate. Further development of this code will include addition of gas phase reactions and 3-D stress formation within the substrate. The goal is to provide design and operational guidelines for use of catalytic combustors in power generation facilities.

**André L. Boehman**

**Heat and Mass Transfer in Combustion and Pollution Control Systems**

André L. Boehman’s research interests involve the study of combustion and pollution control systems for applications ranging from automobile catalytic converters to coal-fired power plants. The research efforts have included the development of experimental facilities designed specifically for the study of pollution control catalysts and numerical models for the dynamic behavior and stress formation within catalytic combustors. The research also involves the development of advanced catalysts for use in diverse applications including diesel oxidation and lean NOx catalysts and NOx abatement systems for industrial coal boilers. Further development of this code will include addition of gas phase reactions and 3-D stress formation within the substrate. The goal is to provide design and operational guidelines for use of catalytic combustors in power generation facilities.

**References**


**Keywords**

- pollution control
- heterogeneous catalysis
- combustion systems
Dr. Bitler is currently conducting research in the area of steel processing. Steel used in commercial products such as automobiles is galvanized to reduce corrosion. The two principal techniques for galvanization are zinc electroplating and hot dipping. In order to minimize the cost of this process while creating a durable coating, it is necessary to control the reaction products between the Zn-steel interface.

An electron microscopy study of the reaction between zinc and steel and the products it forms during commercial galvanized steel processing has been performed, and a new sample preparation technique was developed for the industry.

The 8-phase was found to have quasi-crystalline features. Intermediate phases also play an important role in the mechanical integrity of galvanized steels. Bitler's work has been funded by Inland Steel and the American Electroplating Society.

References


Figure 1. 1D lattice image of the 8-phase, and 6D tilt 2D selected area diffraction pattern (SADP) from the image in Figure 1a.

Figure 2: 6D (0001) SADP and 6D (111) SADP.

Keywords

solid-state diffusion, solid-solid reaction kinetics, soft and hard magnetic materials, steel processing, galvanization, electroplating.
Altaf H. Carim
Microstructure at Solid-State Interfaces

Professor Carim's research interests are centered around the microstructure and microchemistry of solid-state interfaces. The present review paper will discuss the transmission electron microscope (TEM). Current studies include an exploration of the dilute carbon contents formed as an interfacial phase during heating of ceramics, and an atomic-level investigation of interfacial structure and defects in oxide superconductor thin films. Some aspects of the latter project are briefly described here.

There are many ways to produce high-quality films of YBaCuO material that was recently found to be a superconductor at temperatures up to about 92 K. For all these deposition techniques however, it is the final microstructure that controls the crystallographic properties. Orientation of the films is critically important, as the number and nature of crystallographic defects such as stacking faults, grain boundaries, phase boundaries, and dislocations.

High-resolution transmission electron microscopy (HREM) allows us to image individual atomic columns in a sufficiently thin sample. Specific defects and atomic arrangements as interfaces can thus be directly observed on the subatomic scale.

An example of a structure in which stacking faults and dislocations are associated with a particular type of grain boundary is shown in Figure 1. Although high-resolution microscope graphs appear to represent the atomic columns that are viewed as a simple black or white dot, the actual correlation of the images to the atomic positions is often more complex. Formed as a result of the HREM images can be generated based on the atomic structure of the sample and a knowledge of the microscope parameters and operating conditions. By comparing the experimentally obtained images with such simulations, one can determine the terminating HREM images can be obtained through the determine the terminating HREM images can be obtained through the correct displacement associated with defects.

Identification of interfacial phases and defects is important for understanding current flow and for optimizing processing of superconductor thin films. These crystallographic issues, however, are vital for a much wider range of materials as well. For example, the adhesion and mechanical strength of ceramic-metal joints are critically dependent on the microstructure in this solid-state interface. The fracture toughness and high-temperature stability of structural microcomposites are also governed by mechanical constraints. Investigations of interfacial structure can help elucidate the fundamental origins of many materials properties and may suggest how to tailor the processing of real materials in order to improve their performance.

References

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Keywords
chemical formation of ceramics and composites, ceramics, bioceramics, biocomposites, multicomponent phase equilibria, high temperature synthesis
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 polyolefins via borane monomers and transition metal catalysts. It is known that the incorporation of functional groups to polyolefins is a useful method for modifying the chemical and physical properties of polymers (e.g., adhesiveness, compatibility, and durability). However, functional groups containing polymers normally 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 interconversion of borane monomers and polymers. Borane species have been found to be stable to a wide range of transition metal catalysts during polymerizations. In turn, the borane polymers are easily converted to a variety of other functionalities under mild reaction conditions. A broad range of polyboranes, such as PE and PP with various functional groups (e.g., OH, NH2, and halides), have been prepared. Several of the borane-containing polymers have also been used for the preparation of block and graft copolymers. The borane copolymers 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 hydrophobic and hydrophilic polymeric segments. Several interesting graft polymers consisted of polyoxypropylene, poly(1,2-oxazoline), and poly(alkylene oxide) as the skeletons, and several free radical polymers, such as PMAA, PVAc, PAN, have been obtained at the same chain. Several applications of the resulting new polymers have also been investigated in our laboratory, such as the immobilized catalyst using functionalized polyboranes as the supported materials. The catalyst can be recovered and reused for many reaction cycles. The functionalized and grafted polyboranes copolymers are very effective interfacial materials to improve the compatibility in polymer blending, blends, and composites. By using our copolymers, several new high-impact plastics and composites have been prepared. We are also extending the boron-containing copolymers to prepare boron-containing carbon fiber which could have initial stability at high temperature.

References

Figure 1. versatility of borane-containing polymers is functionalization of polymers.

Keywords
polyolefin, borane polymer, block/ graft copolymer, immobilized catalyst

References
Michael M. Coleman  
Multicomponent Polymer Systems

Michael M. Coleman is interested in the application of vibrational (infrared and Raman) spectroscopy to the study of multicomponent polymer systems. In favorable cases, the free-group geometrical interactions are often observed in the infrared spectrum, which can then be related to the specific interactions between polymer chains and the interassociation of two polymers of a binary blend. With information on the free energy of mixing of systems that has been developed using an atomic model, Coleman's group has been able to predict phase behaviors, molar quantities, and maps for a wide variety of polymer blends. Extension to more complex systems, such as ternary blends and copolymers containing multiple specific interaction sites, are currently being studied.

Ralph H. Colby  
Polymer Dynamics, Rheology of Polymer Melts, Blends, Solutions, Gels, and other Complex Fluids

Using rheological techniques to experimentally probe the dynamics of polymer liquids is the thrust of Dr. Colby's research program. Simple notions of scaling are used to construct models for polymer dynamics, allowing for interpretation of the rheology data. Current interests include polyethylene terephthalate, liquid crystalline polymers, blends, block copolymers, miscible polymer blends, branched polymers, networks of both charged and uncharged polymers, surfactants, and colloidal suspensions.

In many cases, polymer dynamics are controlled by the motion of individual chains. In these cases, time scales longer than the time it takes for molecules to diffuse a distance equal to their size, the material flows like a simple liquid. However, when there is large-scale structure present in the fluid (such as in liquid crystalline polymers or surface-active solutions) viscoelastic response is evident on time scales much longer than the molecular diffusion time.

An example of this is shown in Figure 1, which plots oscillatory shear data for a liquid crystalline polymer. In this experiment, the frequency of the mechanical oscillation is varied, so as to probe the response of the polymer on different time scales. The arrows indicate the frequency corresponding to the reciprocal of the molecular diffusion time. In its nematic phase (solid curve), the viscoelastic response is liquid-like at frequencies smaller than the frequency for molecular diffusion (reflected in the fact that the high modulus G' is dominating the response at low frequencies).

In contrast, the smectic phase (open symbols) is still highly viscoelastic on time scales much longer than the molecular frequency for molecular diffusion (because the storage modulus G' is comparable to G' at low frequencies). The smectic structure apparently gives rise to viscoelastic response of this polymer on long time scales. We are currently designing experiments to explore the relation between structure and properties of similar systems in a systematic fashion.

References

Figure 1: Oscillatory response of a liquid crystalline polymer in its smectic phase at 24°C (open symbols) and in its nematotic phase divided at 34°C (solid curve). The arrow indicates the reciprocal of the time it takes for the polymer to diffuse a distance equal to its size.

Figure 2: Spectra of polyester (EMA/PE) blends

Keywords
polymers, blends, phase behavior, polymer rheology, spectroscopy, hydrogen bonding, micellar polymer blends, phase behavior, polymer rheology, spectroscopy, hydrogen bonding

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Keywords
polymer physics, rheology, viscoelasticity, structured fluids, complex fluids, scaling models
The optimization of processing parameters to properly control gas-metal reactions at metallic surfaces, internal reactions at interfaces in metals and composites, and the redistribution of elements in alloys is essential to the improvement of existing structural materials as well as to the development of materials needed to meet demands for high-temperature strength and corrosion resistance.

Such studies require a high degree of parameter control to clearly separate the effects of the several process variables and to establish the controlling mechanisms. Because this degree of constraint is rarely realized in commercial operations, laboratory procedures must be developed that can readily be translated into industrial applications—a step that is frequently overlooked at the interface between science and technology. The scope of each study is quite broad, ranging from the effects of the heating environment upon the formation of surface compounds that influence diffusional processes, apparitions, and properties, to the effects of micro levels of impurities on the transformation products developed in alloy steels.

One such example is an examination of the interaction of species that form during gas-metal reactions. Figure 1 illustrates the decrease in weight gain of 316 stainless steel as the oxidizing potential of the nitrogen-base annealing atmosphere increases. This apparent contradiction arises because the primary cause of weight gain in this instance is not oxide formation, but is due to the formation of internal nitrides. Nitride formation is suppressed with the increased formation of an oxide film which inhibits diffusion of nitrogen across the gas-metal interface.

Lee J. Cuddy

Effects of Compositional and Processing Variables on the Structure and Properties of Wrought and Powder-Processed Alloys and Metal-Matrix Composites

References


Figure 1. 304L Weight Change vs. pO2

\[ \Delta W, \ mg/cm^2 \]

\[ \log (pO_2, \ atm.) \]

0.2

0.3

0.4

0.6

0.8

1.0

1.2

-21

-20

-19

-18

-17

Keywords

gas-metal reactions, processing parameters, interfaces, element redistribution in alloys

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Semih Eser

Carbonization, Mesophase Development, Carbon Deposition, Coal Swelling under Pressure

Semih Eser is carrying out research on carbonization of petroleum feedstocks, microscopic characterization of solid carbons, solid carbon deposition on metal and carbon surfaces, thermal degradation of hydrocarbons under superelevated conditions, and coal swelling under high pressure in reactive environments.

Delayed coking of the petroleum-heavy feedstocks (e.g., the bottom of the barrel of crude oil or heavy ends from catalytic and thermal cracking of petroleum fractions) produces light distillates (e.g., gasolines and kerosenes) and petroleum coke. Depending on the microstructure and composition, petroleum coke can be used for (1) manufacturing graphite electrodes to produce steel in electric arc furnaces, (2) making anodes used in aluminum production or in other electrolytic processes, (3) burning to raise industrial steam without producing ash.

The most significant process that takes place during carbonization in a delayed coker is carbonaceous mesophase development. The structure and properties of the solid carbons produced by thermal treatment of hydrocarbons (e.g., graphite electrodes and carbon fibers) can be controlled principally by the characteristics of the carbonaceous mesophase formed during low-temperature carbonization. Carbonaceous mesophases have properties similar to those of nematic liquid crystals, and it is easily characterized by polarized-light microscopy. Figure I shows a polarized-light micrograph of carbonaceous mesophase from a decaent-oil sample, indicating the stabilization of anisotropic mesophase spheres that coalesce to form anisotropic solid carbon structures. A high degree of anisometry on a well-developed mesophase in the form of elongated microstructures is required to manufacture high-performance graphite electrodes on carbon fibers.

A major challenge in the coking industry has been the establishment of basic relationships between the chemical constitution of the coke feeds and the microstructure of the resulting coals. The complexity of the feed streams has forced the researchers to use averaged data from spectroscopic techniques such as n.m.r. and FTIR. Our work is focused on identifying the molecular species present in coke feeds, particularly in heavy oils, which are used for producing highly graphitizable pyrolysis petroleum coals called socalled coals. Chromatographic separation techniques such as column chromatography, thin-layer chromatography, and high-performance liquid chromatography in conjunction with GC/MS and high-resolution MS have been useful for determining the molecular composition of decaent oils. This information, in turn, allows us to seek correlations between the molecular makeup of the feeds and the quality of the resulting coals.

A rationalization of such correlations is possible through understanding the relationships between the molecular parameters of the aromatic hydrocarbons and the mesophase development and carbon deposition.

References


Figure 1. Polarized-light micrograph of a solid produced by carbonization of a decaent oil, indicating the mesophase spheres and their coalescence to form anisotropic structures.

Keywords:
- Carbonization, Mesophase Development, Carbon Deposition, Coal Swelling under Pressure
- Anthracite and phenanthrene have shown that the kinetics and chemistry involved in the formation of large molecules is closely related to the mesophase development during carbonization. The substantial differences in the reaction mechanisms, kinetics, and mesophase development during carbonization of these two materials have been related to the differences in their electronic structures.

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Baysens:
- Chemistry of carbonisation, mesophase development

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Professor Gordon is interested in controlled polymer architecture to achieve specific properties. His current research program includes controlling molecular architecture by the use of degradable carboxylic initiators for anionic polymerization, the synthesis of new bio-medical materials to control diffusion of water in the Penn State artificial heart, and the synthesis of polymers that degrade in the environment after their useful life.

Anionic initiation can be used to accurately control the molecular weights and the shape of a polymer chain. The chain can be formed in a linear, star, or cyclic form. By the use of controlled initiators we have prepared all of these structures including a new cyclic polymer that can be cleaved by treatment of mild acid. New macromonomers have also been prepared that greatly change the properties of pressure sensitive adhesives.

The Penn State Heart is made of nearly all plastic materials. One of the many crucial parts is the blood sac that pumps the blood. The sac is designed to be an elastomer and has to have a surface that is compatible with blood. Currently the best material available is a segment block copolymer that is made up of polyurethane/urea and poly ethers. This material is ideal except that water vapor easily diffuses through the material and then condenses in the mechanical bearing around the motor. Filling the space where the pump works. A polymer science solution is being worked on to eliminate this problem of the water. We have synthesized a new polymer that has similar polyurethane/urea segments to the currently used material and still rubbery segments that can extend barriers to water vapor transmission. The material shows greater than an order and 1/2 decrease in water vapor transmission.

Polymers in the environment have become a critical social issue. We have developed a new route to make polymers degradable. By making copolymers of PET, a common commercial polymer, with esters that are easily hydrolyzed, we have made a family of polyesters that have physical properties of PET, yet degrade over several years by reaction with water in the air.

Keywords
polymer synthesis, controlled architecture, anionic polymerization, bio-medical polymers, biodegradable polymers, polymer degradation
Ian R. Harrison  
This Films for Long-Duration Balloon Flights

Developing and utilizing an understanding of mechanical properties in space-rated polymer films is the focus of Dr. Harrison's research, which is currently being supported by NASA. Such films are approximately the thickness of a human fingernail, yet they are sufficiently strong to support an astronaut's weight or to construct balloons that can carry payloads of up to 10,000 pounds to altitudes of nearly 150,000 feet. When fully inflated, these balloons are several miles in diameter, and are composed of layers of film that are assembled with approximately two feet of seal. The balloons are used as tools for conducting experiments in high-energy physics on atmospheric science, for instrument and monitoring circuit deploys.

Harrison's contribution lies in understanding how processing and polymer structures interact to influence the mechanical properties. Such an understanding is crucial in trying to produce films that are tougher and more resistant to deformation. The next generation balloon films are earmarked for the extended flight times required for future scientific payloads.

Current efforts are directed in three areas: (1) production of a molecular-level model that can explain film physical properties; (2) testing, evaluation, and modification of semi-commercial films; and (3) production of unique blends of existing polymers. Modeling involves integrating a large amount of characterization data into a comprehensive and consistent structural picture. This part of the study is approaching completion, the model is being "fine tuned" and key tests performed to check its validity. Incidentally, commercial film and the model studies are conducted with films formed by a blown-film process (Figure 1). There are a large number of process variables associated with this particular technique that makes the task quite difficult.

Contacts with industry have been very useful. A number of manufacturers have made suggestions and tested and supplied variations of their standard materials in order to advance the project. Progress in understanding will continue to benefit from interaction with this research at Penn State, yielding a more comprehensive picture of the structure-property relationships produced by controlled variations in the blown-film-processing operation.

References

Figure 1. Schematic of the blown-film process.

Keywords
structure-property relationships in polymers, thermal properties, blown films, elongational rheology, polyethylene, TREF

David J. Green  
Mechanical Behavior of Brittle Materials

References

Figure 1. Schematic of the blown-film process.

Keywords
mechanical behavior, brittle materials, failure analysis, micromechanics, fracture mechanism, structural reliability

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Keywords
structure-property relationships in polymers, thermal properties, blown films, elongational rheology, polyethylene, TREF
Patrick G. Hatcher
Organic Geochemistry of Macromolecules in Fossil Fuels and the Modern Environment

lachter is involved in a multidisciplinary field of organic geochemistry with a focus on coal, studies of humic materials, and the chemistry of kerogen from ancient and modern sediments. In addition, his interests include applications of nuclear magnetic resonance and analytical pyrolysis to the study of ancient and modern sediments and the process of humification. By using remnants of plant fossils in the ground, Dr. Hatcher's research team can gain an understanding of the chemical changes that occur in the fossilized plant remains. His research involves determining the structure and function of the plant remains at various stages of transformation or fossilization. The three-dimensional structures of these plant remains are visualized using both newly acquired and existing imaging techniques. The imaging techniques used include electron microscopy and X-ray diffraction. The three-dimensional structure of the plant remains is then used to study the chemical changes that occur in the fossilized plant remains. The chemical changes that occur in the fossilized plant remains are then used to study the physical properties of the fossilized plant remains. The physical properties of the fossilized plant remains are then used to study the chemical changes that occur in the fossilized plant remains.

Figure 1: A three-dimensional image of coalified wood obtained by magnetic resonance imaging.

References

John R. Hellmann
Development of Materials with Tailored Properties

Professor Hellmann’s research interests focus on the development of new materials and composite materials. He integrates methods for the utilization of structural and chemical properties of these materials in high-performance applications. These research efforts go beyond the range of conventional composite and inorganic materials. Effects of microstructure on the thermal, mechanical, and electronic properties of materials are basic to the fundamental interest in these materials. Recent studies in Professor Hellmann’s laboratory address tailoring of interfacial layers in novel ceramic and metal matrix composites to enhance high-temperature fracture toughness and creep resistance. His research team’s development of new methods of fabrication for materials with unique properties continues to expand. This program is unique, and opens a myriad of possibilities for producing advanced ceramic-composite materials with high-temperature structural components for the aerospace, automotive, and industrial-heating systems. Current efforts are concentrating on the selection and application of fiber compositions to achieve the levels of structural and 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 developing new composites for structural and medical applications. His research group includes the determination of the critical size of defects for predicting the enhanced fracture toughness and creep resistance of materials. The research group is also developing new methods for fabricating advanced composite materials with tailored microstructural characteristics. His research group has combined finite element analysis with experimental verification of interfacial toughness behavior to assess the relative contributions of thermomechanical stress and applied mechanical stress to the fracture behavior of the interfacial failure of fiber reinforced composites. Results of these efforts have been instrumental in identifying new composite compositions contributing to improved fracture toughness as well as in establishing criteria for properly quantifying the contribution of the interfacial toughness of the interfacial fracture process. Much effort has been devoted in his laboratory to developing new testing methods for investigating the behavior of these important materials to temperatures as high as 1500°C in controlled environments.

Data compiled in Hellmann’s lab on the temperature-dependent properties of these 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 been conducted with applied and supported development activities. Results of these efforts and applications in systems and component design are detailed in several technical papers on the development of advanced materials for high-temperature industrial, aerospace, and automotive applications.

References

Figure 1: Longitudinal section of a silicon carbide/ceramic-matrix composites made by infiltration techniques developed in Hellmann’s laboratory.}

Key words: ceramics, intermetallics, composites, interfaces, coating, mechanical properties, thermal properties, processing, microstructure, structure-property relationships
Donald A. Koss
Interfacial Shear in Metallic Matrix Composites

A key issue in designing high-performance structural materials is optimizing both strength and fracture resistance. Metallic matrix composites provide a good example of new ways to tackle this old problem. For example, reinforcing a matrix with well-bonded, aligned, strong fibers will likely impart good strength in a composite. However, improved fracture resistance is usually obtained if the interface/matrix interaction is properly bonded, allowing fracture energy to be consumed by crack deflection or interface shear during fiber pullout. Thus, the fiber-matrix interface shear behavior is an important aspect in deforming composite performance.

The importance of fiber/matrix interfacial shear behavior in controlling both the strength and the fracture behavior of fiber-reinforced composites has resulted in many studies directed at determining interfacial failure response. In metal matrix composites (MMCs), as well as intermetallic matrix composites (IMCs), the combination of chemical bonding and thermally-induced clamping, due to the thermal expansion mismatch between the fiber and matrix, usually results in high interfacial shear strengths, especially at low temperatures. While this is good for strength, many of the high-performance matrix materials have intrinsically poor ductility and require some form of fiber pullout for improved toughness. Unfortunately, significant fiber pullout occurs only under conditions of low interfacial shear strengths. Thus, we are studying both the methods by which interfacial shear strengths may be controlled, and the methods of determining interfacial shear behavior. Our research focuses on high-temperature composites using sapphire-reinforced NiAl, TiAl, and Nb composites as model systems. Both experimental studies and computational modeling are being used to understand the interface behavior during loading.

References

Figure 1. Influence of fiber/matrix interfacial shear strength on intermetallic matrix composite failure behavior. (a) Non-coalescing and (b) interfacial failure.

Keywords
deformation and fracture, composite materials, intermetallic alloys, powder processing

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Keywords
deformation and fracture, composite materials, intermetallic alloys, powder processing
The development of chemistry and corrosion sensors for thermal power plants is one research project currently being conducted by Dr. Macdonald. This project, undertaken in cooperation with the University of Pennsylvania for a Spanish utility, aims at developing sensors to measure in situ corrosion potential, crack growth rate, general corrosion rate (via the analysis of electrochemical noise), solution conductivity, and the concentrations of hydrogen and oxygen in power plant heat transfer fluids at temperatures up to 550°C. Dr. Macdonald and his group believe that the sensors will revolutionize chemical and corrosion control protocols in thermal and nuclear power plants because of the much tighter control that will be possible over plant operating conditions.

The first phase of the project involves the development and setting of the various sensors (for example, the fracture monitor in Figure 1). Later work will involve the installation and operation of the sensors in a Spanish power plant.

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

References

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Keywords
polymer, surface, thermodynamics, statistical mechanics, neutron scattering and reflectivity, semicrystalline polymers

Figure 1. An optical micrograph of a phase separation phenomenon in a triblock (50:50:50) polymer mixture.

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

Figure 1. Schematic of an advanced fracture monitor:

Keywords
mechanical and physical properties of ceramics, composites, electrochemistry, corrosion, high-temperature aqueous systems
Gary L. Messing  Ceramic and Particulate Materials Processing

The fabrication of advanced ceramics with targeted properties requires control over all process steps from powder synthesis through sintering. The complex relations between the myriad processes encompassed in ceramic processing is the general focus of Prof. Messing’s research program. For example, he and his group have had a sustained effort for many years to understand how to regulate ceramic phase development through the application of fundamental concepts of phase stability. Using seed crystals or by developing self-nucleating sol–gel chemistries, they have demonstrated unique control of phase development, transformation kinetics, sintering, and microstructure development in alumina, silica-based ceramics, and multilayer.

Spray pyrolysis is a unique process for the synthesis of advanced ceramics films from spray 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 aerosol atmosphere particulate materials and films of mixed metal oxides ceramics, nonoxide composite materials, and metals can be prepared.

Figure 1. Schematic of spray pyrolysis system.

References

Keywords
ceramic processing, powder synthesis, spray pyrolysis, solid-phase epitaxial and phase transformations, sol–gel, sintering
Robert E. Newham

"Smart" and "Very Smart" Ceramics

Robert E. Newham is Alcoa Professor of Solid State Science, and Associate Director of the Materials Research Laboratory. Recently elected to the National Academy of Engineering, Newham has written nearly 400 research papers on electrorheology and composite materials for electronic applications. During the past year, he was awarded the Centennial Prize by the Ceramic Society of Japan, the John Ippen Medal of the American Ceramic Society, and the First International Ceramic Prize of the Academy of Ceramics for "distinguished and creative contributions to the advancement of ceramic science and technology, especially in the field of composite ceramic electronics." Newham is active in several professional societies, having served as editor of the Journal of the American Ceramic Society, President of the American Ceramic Society, and Distinguished Lecturer for the Institute of Electrical and Electronic Engineering.

His current research program is centered on "smart" and "very smart" ceramics. Smart ceramics are defined with reference to the sensing and actuating functions of living systems. A smart ceramic senses a change in the environment, and using a feedback system, makes a useful output response. It is both a sensor and an actuator. Applications include vibration damping systems for space structures, and energy-saving winter/summer controls for homes and factories. 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 defini-
tion can be extended to a higher level of in-
telligence: a very smart ceramic senses a change in its surroundings and responds by changing one or more of its property constants. Such a very smart material can tune its sensing and actuating functions in time and space to optimize behavior. The relationship between smart and very smart materials is essentially one between linear and nonlinear properties. The physical properties of some materials can be adjusted by bias fields or forces to control response.

Newham is currently developing a family of "very smart" transducers, which utilize the nonlinear properties of relaxor ferroelectrics interlaced with thin layers of rubber and metal end caps. The basic design is patterned after megalinear ceramic composite actuators developed in his laboratory (Figure 1). Shallow cavities positioned between the metal caps and the ceramic disk can be controlled to induce the radial displacements of the piezoelectric ceramic to the large axial motions of the metal end caps (Figure 2).

Five important characteristics of an elec-
tromechanical transducer are the resonance fre-
quency $f_r$, the mechanical damping coefficient $D$, the acoustic impedance $Z_a$, and the electrical impedance $Z_e$. In the tunable transducer, the magnitudes $f_r$, $Z_a$, and $Q$ are controlled by stressing thin layers of rubber, while $k$ and $Z_e$ are manipulated by applying bias fields to piezoelectric layers of relaxor ferroelectric such as magnetostrictive PZT. As shown in Figure 2, electrostrictive PZM gives larger strains than the usual PZT transducers.

The search continues for "smarter" ceramics for use as sensors and actuators. The nonlinear properties of very smart materials are often associated with nanoscopic structure and diffractive phase transformations. Under these circumstances the structure is poised on the verge of an instable condition, and responds steadily to external influences such as electric or magnetic fields, or mechanical stress.

References

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References


Kwadwo Osseo-Asare

Aqueous Systems, Materials Processing, Hydrometallurgy, Separation Science, Materials Synthesis, Dissolution Processes, Colloids and Interfaces

References


Figure 1. TEM micrograph of colloidal particles in the NP-3 (polyacrylamide)/water microemulsion. [NaCl] = 4.4 x 10^-4 M; [NaOH] = 1.2 x 10^-4 M.

400 nm

400 nm

Paul C. Painter

Effects of Strong Intermolecular Interactions on the Properties of Polymers

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 as water, alcohol, amine, etc., that form hydrogen bonds. At an early stage, the assumptions of simple models, such as regular solution theory, were recognized as invalid 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 is treated by using the assumption of a chemical equilibrium between the monomaurals of the associated species, and this approach has formed 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, boiling of mixing). In collaboration with Dr. Michael Coleman, Painter has sought to do the same thing, to adapt this approach to a description of the phase behavior of polymer mixtures, and further, 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.

References


Figure 1. Hydrogen bonding in poly(vinyl phosphonate).

Keywords:

aqueous systems, materials processing, hydrometallurgy, separation science, interfaces and colloids.

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Keywords:

hydrogen bonding in macromolecular systems (synthetic polymers and co-polymers); polymer blends; gel; liquid crystal/polymer mixtures; coal structure.
Sarma V. Pisupati

Emissions Control from Stationary Combustion Systems

Dr. Pisupati's research interests are primarily in studying the effects of properties fuels on combustion behavior and the effects of fuel characteristics on the formation and emission of pollutants from the products of combustion. Specific research topics include: a) the effect of oxygen concentration on the formation of nitrogen oxides; b) the effect of fuel properties on the formation of sulfur oxides; c) the effect of fuel properties on the formation of particulate matter; and d) the effect of fuel properties on the formation of volatile organic compounds (VOCs). Dr. Pisupati has made significant contributions to these areas and has published numerous papers on these topics.

References

Durov Experience of Natural Weathering and Laboratory-Catalyzed Brucite Oxidation.


Effect of Weathering and Laboratory Acceleration on Soot Agglomerate and Combustion Behavior. Proc. 22nd Conf. on Combustion Behavior.

Fuel 75(4): 621-630.


Soot Behavior of Circulating Fluidized Bed Combustion. The Role of Thermodynamically Induced Fuels. Proc. 22nd Conf. on Combustion Behavior.


Figure 1: Schematic diagram showing the mechanism of soot formation and growth in a fluidized bed combustor.
Howard W. Pickering

Professor Pickering's teaching and research activities focus on the scientific and industrial implications of the corrosion of metals and methods for its prevention. The relevance of electrochemical (oxidation and reduction) and gas-phase reactions, and the changes that the metal surface undergoes during the reaction, are also of interest. More specifically, research in our corrosion laboratory includes the study of (1) selective element dissolution from alloys, (2) localized electrochemical-degradation processes such as crevice corrosion, pitting corrosion, and grain boundary corrosion; (3) reduction reactions including hydrogen evolution and its absorption and diffusion into metals; (4) precipitation, segregation, and metal-gas-oxidation reactions using atomic-probe-field ion microscopy (AP-FIM); and (5) surface reconstruction and chemisorption in metal-gas systems and of metal electrodes in aqueous solutions using scanning tunneling microscopy (STM) and atomic force microscopy (AFM).

References


Figure 1: A photograph (a), and schematic (b) of the corrosion showing the effect of the stress power on pressure. The corrosion can be categorized into:...

Keywords

surface properties; corrosion and oxidation of metals; electrochemical characterization; scanning tunneling microscopy; atom-probe FIM

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Professor Randall’s research interests are in processing of semiconductor properties in advanced electronic materials. Special attention is given to problems in the application of remote and in-situ techniques to achieve novel architectures at fine scales. We are investigating the use of electrical fields to assemble nanoscale components in composite and thick film form. In general, when an electrical field is applied to a stable particle suspension, the particle motion is precisely dictated by dielectrophoretic and electrorheological forces. Dielectrophoretic assembly involves the induction of a dipole-dipole interaction that destabilizes the system in such a way that the particles undergo uniaxial agglomeration along the electric field direction. This process has been employed to fabricate multitudes of materials that undergo in situ polymerization to prepare unique composites with dielectric anisotropy.

Electrostatic deposition exploits an electric surface charge on particles in suspension migrating in the presence of an appropriate electric field to form a composite. When the particles are in high-speed streams, the composite material is formed in a sheet. By understanding the colloidal stability, the deposition kinetics and the suspension stirring issues we have fabricated 1–10 micrometer BTO-TiO2 thick films with high dielectric constant and low losses comparative with other thick film technologies. The ongoing work is focused on establishing the scientific and engineering aspects of the deposition process. Electrostatic deposition of cerium oxide particles are used to give potential advances in a number of applications, including piezoelectric materials, biomedical ultrasound probes, and interconnection chemical sensors.

Ferroelectric and related materials are of interest due to their unique anisotropic properties that are being used in piezoelectric, electroacoustic, pyroelectric, and capacitive applications. Our group has focused attention on the role of mesoscopic structures on physical properties. Recent work using novel techniques for transmission electron microscopy and neutron scattering on the zinc blende structure has been on the growth strain effects on domain switching mechanisms during poling and defect inclusion spatial modulations within domain structures, each of which shows a strong dependence on the electric field properties and leakage currents.

Keywords: Optoelectronics, Impedance measurements, transmission electron microscopy, composites, thick films

Figure 1. Planar abstracts, dielectric constant and<br>thickness dependence of Al2O3-TiO2 membranes in Ti-doped TiO2.

Figure 2. Temperature dependence of Al2O3-TiO2 membranes in Ti-doped TiO2.
James P. Runt

Chemically Dissimilar Polymer Mixtures

Mixtures of chemically dissimilar polymers are of considerable technological importance compared to traditional single-component systems because of their potential for superior mechanical and physical properties. A particularly important class of these polymer blends are those that contain high-performance, crystallizable polymers. In general, Dr. Runt's research has focused on developing a fundamental understanding of crystallization and phase behavior in these and other multiphase polymer systems, and their relationship to ultimate properties. Some specific research topics of current interest include co-crystallization in homopolymer/copolymer mixtures, and the use of dielectric measurements to probe local molecular environments in multicomponent systems.

In semi-crystalline polymers, the existence of order-disorder interphases between the crystalline and amorphous phases was predicted several decades ago and subsequently confirmed experimentally. Such interphases are also of prime importance in mixtures containing crystalline polymers, but poorly understood. The focus of this part of Runt's research has been to explore the interfacial regions in semi-crystalline binary polymer blends using experimental techniques such as small-angle scattering and measurement of the relaxation behavior.

References

Figure 1: Schematic of three possible microstructures of a miscible binary blend of an amorphous (---) and semi-crystalline (- -) polymer. A, amorphous polymer is kinetically B, intercrystalline C, interphasites.

Keywords
phase behavior and crystallization of polymer blends; interphases in crystalline polymer blends; fatigue and microstructure in crystalline polyblends: quantitative microscopy of polymer fracture surfaces and polymer/interfacial composites; dielectric spectroscopy.
The impact of fossil-fuel use on the global environment is greater than that of any other source of carbon emissions. The main sources of carbon emissions are coal, oil, and natural gas. Fossil fuels are used in power generation, in the production of chemicals, in transportation, and in many other industrial processes. The burning of fossil fuels releases large amounts of carbon dioxide, which is a greenhouse gas that contributes to climate change.

To reduce greenhouse gas emissions, many countries are investing in renewable energy sources such as wind, solar, and hydroelectric power. These technologies are becoming more cost-effective and are increasingly being used to meet energy needs. Additionally, measures are being taken to improve the efficiency of fossil fuel use, such as through the development of cleaner-burning technologies and the use of carbon capture and storage (CCS) methods.

In conclusion, the continued use of fossil fuels poses significant risks to the environment and public health. However, by investing in renewable energy and improving the efficiency of fossil fuel use, we can reduce our reliance on these harmful fuels and work towards a more sustainable future.
Molecular Beam Epitaxial Growth of Oxide Thin Films

Harold H. Schobert
Fuel Formulation

Advanced generation (high-Mach) aircraft will generate significant heat in the airframe and "skin" as a result of elevated heating. One solution to this problem is that the aircraft's fuel might serve as a heat sink to cool hydraulic fluids, sensitive electronics, and other aircraft components. The thermal stressing of the fuel in such situations can cause pyrolytic decomposition, leading to the formation of solid carbon deposits. If these deposits plug fuel lines or burners nozzle in the engine, caustrophobic could occur. Because thermal stresses envisaged for advanced aircraft are well above the range in which price fuel stability studies have been conducted for conventional aviation fuels, the goal is to develop a fuel formulation that will withstand temperatures of 900°F for two hours without deposition problems.

Coal-derived jet fuels are more stable in the high-temperature pyrolytic regime than are typical petroleum-derived fuels. The key compositional difference is that higher proportions of fuel synthesis, particularly polyaromatic cyclodimerization, are catalyzed in the coalfuels. For example, tests with pure compounds show that these possess remarkable thermal stability. Because coals have molecular structures based mainly on polyaromatic structures, the potential to produce higher yields of thermally stable jet fuels than if the polyaromatic aromatic structures can be removed chemically from the macrostructure of the coal structure and subsequently hydrogenated to polyaromatic.

Conversion of coal to jet fuels and other useful liquid products requires careful adjustment of reaction conditions and use of catalysts that can break down the coal structure, hydrogenate the high-molecular-weight, coal-derived fuel products, or do both. Recent and current work on development of liquefaction catalysts includes studies of metal-impregnated C8, tar-cracker catalysts, and organometallic cluster compounds.

Figure 1. A highly schematic representation of the ME process used to grow an oxide compound (e.g., CuCaO). The stepped beams are individually controlled by changes that control the sequence and quantity of species reaching the growth surface.

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Keywords
jet fuels, coal, coal liquefaction, novel catalysts, coal ash, gasification systems, combustion systems
Physiological and Chemical Characterization of Metal Powders

References


Dr. Song’s research interests include catalysis in fuel processing and coal liquefaction, shape-selective synthesis of specialty chemicals, synthesis and application of novel mesoporous zeolites, and chemistry of high-pressure pyrolysis of hydrocarbons. A major challenge in coal liquefaction research is to convert coal into liquids at lower temperature. Recently, Song’s group has found that water and dispersed Mo3S3 catalysts could dramatically improve coal conversion at temperatures above 325°C – 357°C, which are much lower than those used in conventional processes (400 – 470°C). For example, adding water to catalytic run at 356°C can double the coal conversion, as shown in Figure 1. The promotion effect of water depends on the temperature range and water to coal ratio and catalyst type. Research is ongoing to examine how and whether H2O affects the C-C and C-O bond formation and whether and how H2O affects the activation and passivation of catalytically active phases.

Song’s research on shape-selective synthesis focuses on sodium-catalyzed conversion of polyaromatic hydrocarbons, which has great potential for new and emerging applications. Ongoing work involves catalytic tests on several types of reactions as well as analytical characterization for understanding the relationship between the pore structure and surface acidity characteristics of the catalysts and their activity and stability. The work on selective alkylation aims at adding two alkyl groups on naphthalene to make 2,6-di(ethyl)phenylmethane, and use biphenyl to make 1,4-di(ethyl)biphenyl, which are important building blocks for advanced aromatic polymer materials. There are many possible new products from the alkylation, but only one of them is desirable. The challenge is to control the regioselectivity with reactivity possessing the desired pore structure and surface acidity characteristics.

Recent work concentrated on deamination monoliths that exhibit high selective for isomerization. In an effort to convert phenanthrene into useful chemicals, Song’s group found that simple and Y zeolite could convert the ring-shift isomerization of 1-phenyl-2-naphthalene to 1-phenyl-3-naphthalene. The latter can be used for producing aromatics, which is in demand in the chemical industry. Recent work includes the determination of equilibrium compositions as well as catalytic screening and optimization of the process. The research on low-temperature selective dehydrogenation of naphthalene revealed that mordenite and Y zeolite-supported noble metal catalysts are much more active than the corresponding Al2O3 and TiO2-supported catalysts. Moreover, the trans-decalin to cis-decalin can be selectively produced by catalyzing the cis-decalin composition. A related reaction is the selective dehydrogenation of ethylbenzene to styrene.

Catalysis in Fuel Processing and Shape-selective Chemicals Synthesis

Figure 1. Scheme of an irregularly shaped ≈100 mesh particle a) ≈100 mesh only, b) smaller particles penetrate covers, c) front particles penetrate covers ≈100 mesh particle.

Chunshan Song

Catalysis in Fuel Processing and Shape-selective Chemicals Synthesis

Dr. Chunshan Song’s group has found that molecular H2 dramatically promotes the isomerization of saturated hydrocarbons over some metal catalysts.

More recently, Song’s group has initiated research on synthesis, characterization, and catalytic applications of novel mesoporous zeolites. This work revealed that certain aluminium phosphates are excellent sources for incorporating Al into the silicate framework during hydrothermal synthesis, leading to mesoporous aluminophosphates with good acidity characteristics. Important catalytic applications of the mesoporous zeolite catalysts include low-temperature gasification and hydrodeoxygenation of liquid fuels, and cracking and hydrocracking of heavy oils.

References


Figure 1. Work improves coal conversion in catalytic liquefaction of Wyodak coal using monomer phosphotungstic acid (ATM) as catalytic material at 350°C for 30 minutes under H2 pressure.

Catalysis in Fuel Processing and Shape-selective Chemicals Synthesis

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Keywords: catalysis, coal, coal liquefaction, hydrocracking, coal gasification, aluminophosphates, zeolites, characterization, shape selectivity, specialty chemicals, high-pressure pyrolysis, jet fuel, thermal stability
The chemical mechanisms that govern the nucleation and growth of diamond films from an activated gas phase, and thus the ability to manipulate and control these processes, are not established. The goal of a cooperative research project conducted with Professor Michael Freyaldenhoven is to develop detailed chemical kinetic models that accurately describe the deposition processes. The models include both gas-phase and surface reactions that produce both diamond and nondiamond carbon. The modeling studies are coordinated with experimental programs that include homogeneously nucleated and grown diamond powders from gaseous reactants, and a diamond film deposition process that systematically alternates growth and etching cycles. Experimental and theoretical correlation investigations of nanoscale ceramics are the focus of research conducted with Professor Richard Tessler. Pulse-laser studies were initially performed using single crystals and dense, high-purity CVD diamond films. Current studies on commercially available ceramics are being compared to the base-line data to develop predictive mechanistic models of reaction behavior as a function of microstructure and purity of both the ceramic and gaseous environment. These current efforts have been expanded to include the oxidation behavior of ceramic-oxide composite materials. A related project with Professor Carlo Fantozzi is aimed at developing a fundamental understanding of interfacial reactions in glass-matrix-ceramic composites through experimental studies coordinated with the development of predictive models.

**References**

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Oxidation of alloys outside single-crystal and CVD diamond surfaces. 
In Corrosion and Concrete of Deposited Diamond, 
Transactions, edited by R. Tessler and V. M. Belford. 
Cambridge, MA: The Electrochemical Society.

Keywords:
High-temperature and solid-state chemistry; 
thermodynamics and phase equilibria applied to 
multilayer synthesis and behavior; 
vapor deposition process for diamond and other 
high-temperature materials; experimental and 
theoretical modeling of CVD; corrosion.

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Figure 1: Schematic illustration of the addition of a nanoscale ceramic to a diamond layer. This growth site is identified as a (111) step site. (Freyaldenhoven and Spear, 1988.)
Peter A. Thrower

Carbon–Carbon Composites, Manufacture, Mechanical Properties, and Oxidation Resistance

References


Richard E. Tessler

Degradation of Ceramics, Fibers, and Composites

In many heat-engine, heat-exchanger, and heat-generating systems, advanced ceramics with the requisite thermomechanical properties are thermodynamically 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 scheme can be developed when the processes that control the corrosion and subsequent degradation are understood in detail in terms of rate-controlling reactions and local thermodynamic equilibrium.

The long-term reliability of advanced structural ceramics, ceramic fibers, and ceramic–ceramic composites under static or cyclic stresses at elevated temperatures is of major importance for cryogenic, cryogenic recuperation and cryogenic applications. The understanding of the mechanisms of failure processes and the materials characteristics that control these processes is in the very early stage of development. The design data base of reliable ceramic properties of commercially available materials must be developed to assure optimal application of these materials.

References


Keywords
graphite, carbon–carbon composites, oxidation, boron–carbon compounds

Figure 1. Fracture surface of a specimen fiber tensile tested at 1400°C. There is a region of slow crack growth around the failure origin, e.g., area.

20 μm

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Keywords
point defect and impurity diffusion in silicon and silicon carbide; properties of oxide fibers on silicon or silicon carbide; processing of fibers, composites, and in situ reinforced ceramics: processing, deformation, creep rupture, crack growth.

Figure 2. Fracture surface of a specimen fiber tensile tested at 1400°C. There is a region of slow crack growth around the failure origin, e.g., area.
Troller-McKинstry is interested in the de-
development of electronic ceramics as active ma-
terials and actuators. Her current project is focused on understanding the influence of ferroelectric surface and layer properties. This has led to the development and application of materials that enhance the performance of electronic devices. Ferroelectric thin films are attractive for use in electronic applications, including the development of thin-film sensors and actuators for use in electronic devices. The field of ferroelectric materials has seen significant advances in recent years, and there is considerable opportunity for the development of new materials and applications.

Simplifying the complex behavior of ferroelectric materials, Troller-McKинstry et al. have shown that a thin film of the ferroelectric material PZT can be deposited onto a substrate using a combination of radio frequency sputtering and photolithography. This approach allows for the fabrication of ferroelectric devices with high levels of control over the film properties, which can be tailored to specific applications. The research team has demonstrated the ability to control the thickness and morphology of the deposited films, as well as the ability to integrate these materials with other electronic components. This work has significant implications for the development of next-generation electronic devices.

Peter M. Walsh

Fuel Specification and Combustion Adjustment for Power Plant Optimization

The properties of solid particles formed during combustion of coal and oil in power boilers determine the lifetime of the boiler, the efficiency of the process, and the environmental impact. Walsh and his team have developed a comprehensive understanding of the factors that influence the formation of solid particles during combustion, including the role of fuel composition, combustion conditions, and boiler design. Their research has led to the development of new technologies for reducing the formation of solid particles, thereby improving the efficiency and reducing the environmental impact of power plants.

References


SUGGESTED KEYWORDS

ferroelectricity, spectroscopic ellipsometry, thin films, electronic ceramics

References


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Keywords
combustion, particulate matter emissions, fouling and erosion of heat exchangers
Alter A. Yarbrough

Synthesis and Preparation of Materials

Interdisciplinary Activities

The Intercollege Graduate Program in Materials is an interdisciplinary degree program administered by the Dean of the Graduate School. Faculty members from these colleges—Earth and Mineral Sciences, Engineering, and the Eberly College of Science—and the Intercollege Research Program participate.

The program is designed to accommodate students whose interests span the boundaries of the traditional disciplines. Course and research programs for individual students can be designed to emphasize materials science, materials engineering, or the chemistry or physics of materials.

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SYNTHESIS, DIAMOND, CUBIC BORON NITRIDE, SURFACE CHEMISTRY, CHEMICAL VAPOR DEPOSITION, SOLID-STATE SYNTHESIS, NON-EQUILIBRIUM THERMODYNAMICS

References


Intercollege Research Program in Materials

Dr. David A. Shirley, Professor and Vice Provost and Dean of the Graduate School

The Intercollege Graduate Program in Materials Research Institute (MRI) is an umbrella coordinating organization for the broad and diverse materials research community at Pennsylvania State University. 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 coordinate research in materials science and technology, to provide opportunities for students and researchers in the interdisciplinary field of materials science, to enhance research in materials science, and to foster collaboration among researchers in the field.

The Intercollege Graduate Program in Materials Research Institute is comprehensive and interdisciplinary in nature, and it is interdisciplinary in nature. The program is designed to accommodate students whose interests span the boundaries of the traditional disciplines. Course and research programs for individual students can be designed to emphasize materials science, materials engineering, or the chemistry or physics of materials.
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