materials science and engineering

PENNSTATE

1855

University Park

cover: Polarized light micrograph
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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.

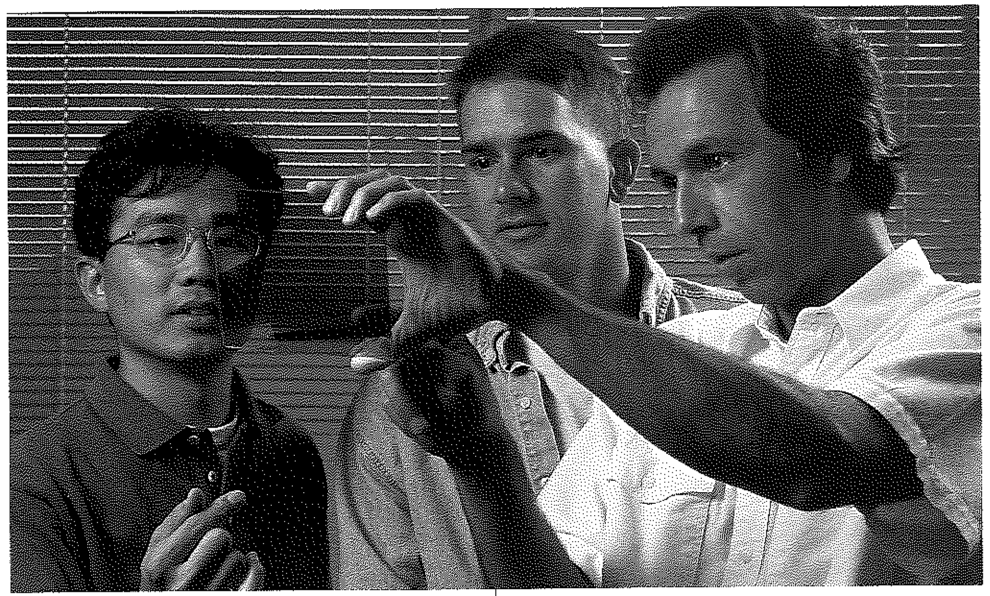
The University Libraries have holdings of about 3.6 million volumes with on-line catalog access. The central Pattee Library is supplemented by specialized satellite libraries, including the College of Earth and Mineral Sciences Library in Deike Building.

partment of Materials Science and Engineering

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 1907–08 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 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 Intercollege Graduate Program in Materials, is administered through the Graduate School.

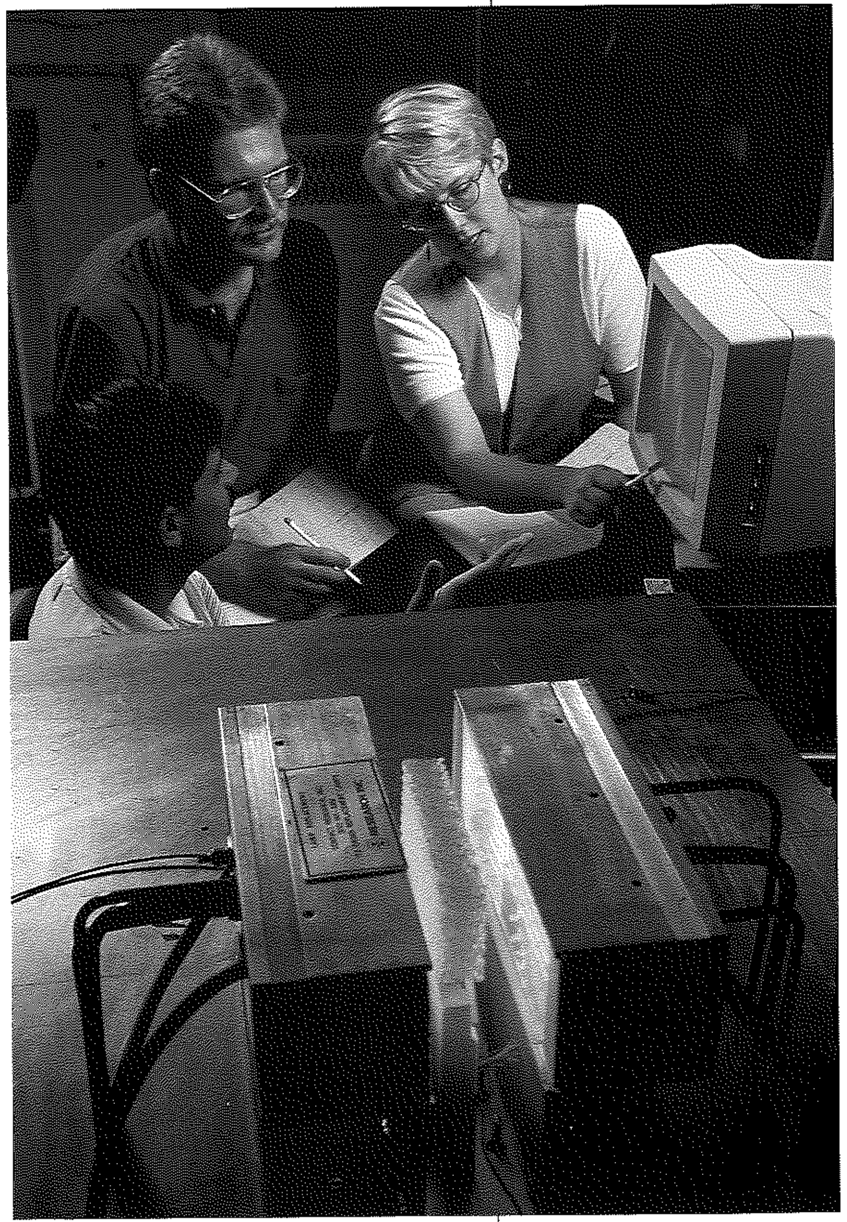
The department is large and diverse, affording students the opportunity to interact with faculty and with postdoctoral and graduate students from a wide spectrum of disciplines. There are forty full-time faculty members, some 200 graduate students, and about 175 undergraduates currently in the department.

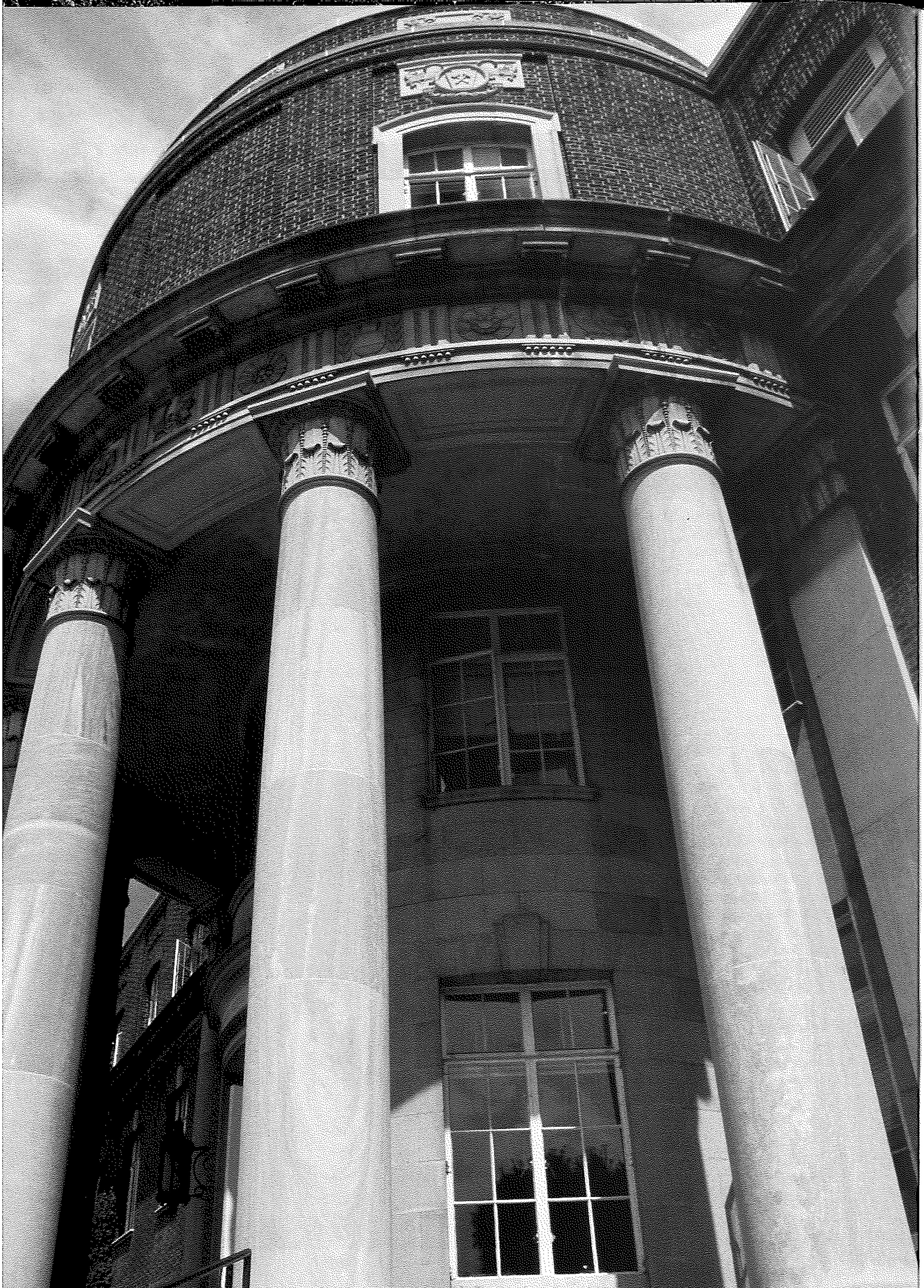


Materials science courses that cut across disciplines are offered, in addition to those in the specialties. Students are encouraged to broaden their horizons by taking these and other University-wide courses.

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 Particulate Materials Center, the Materials Characterization Laboratory, the Energy Institute, the Intercollege 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 as teachers. Eight of the current faculty have won collegewide 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 option depending on the number of openings available and the compatibility of students' interests with current research projects.

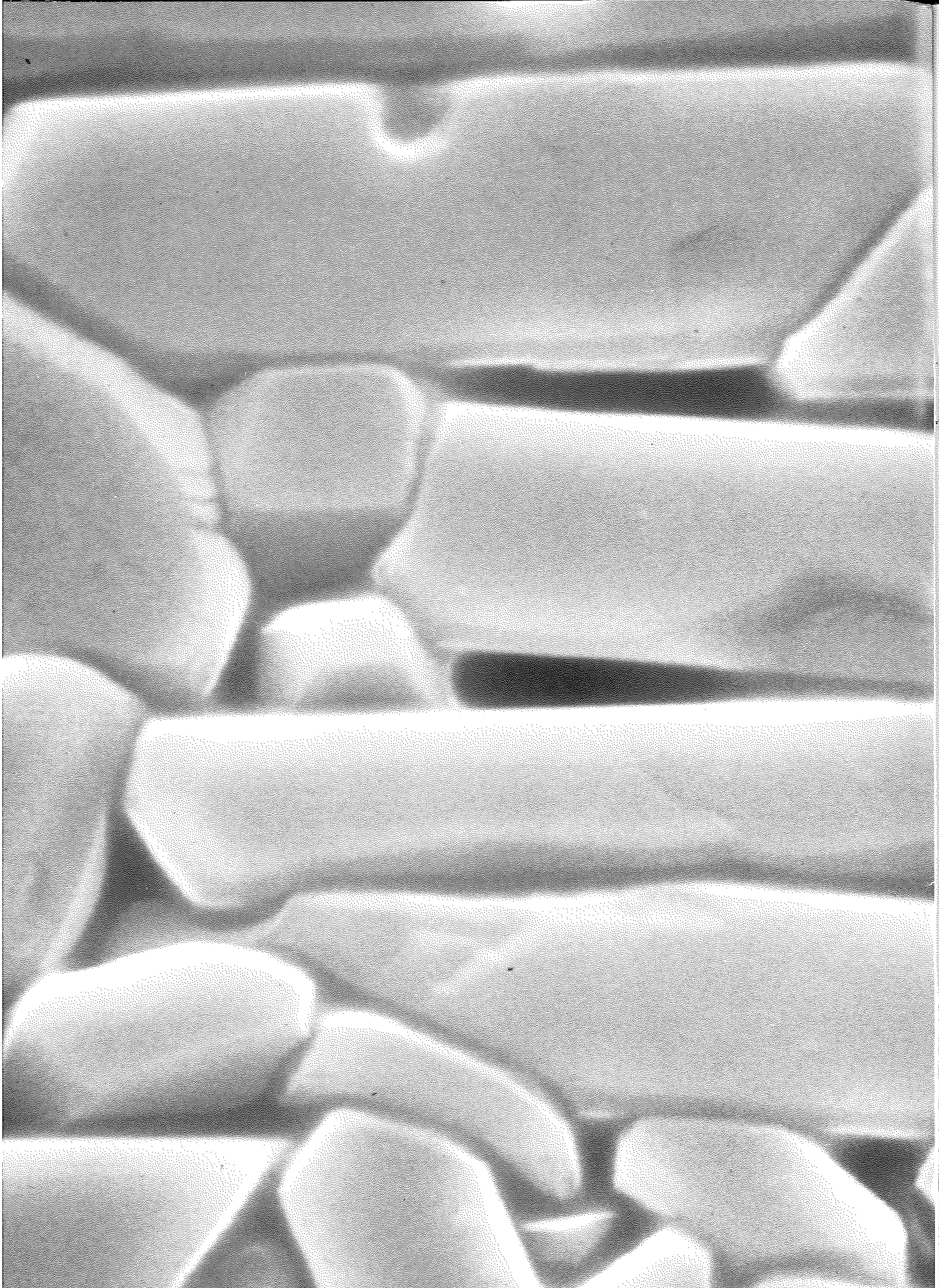
Applicants must have received, from an accredited institution, a baccalaureate degree earned under residence and credit conditions substantially equivalent to those required by Penn State. No fixed minimum grade-point average (GPA) is required for admission, but a junior–senior grade-point average of 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, 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.



Using templated grain growth, platelet-shaped particles of α-Al_{203} are oriented in an alumina matrix during formation and grow

Ceramic Science (CERSC)

DR. DAVID J. GREEN, IN CHARGE OF GRADUATE OPTION

The Ceramic Science specialty covers a wide field with special emphases 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 studies, corrosion studies, and composite materials.

FACULTY

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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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Gary L. Messing, Professor of Ceramic Science and Engineering; Director, Intercollege Materials Research Laboratory; Director, Particulate Materials Center, B.S. (Alfred), M.S., Ph.D. (Florida)

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

Carlo G. Pantano, Professor of Materials Science and Engineering; Director, Materials Characterization Laboratory, B.S. (NJIT), M.E., Ph.D. (Florida)

Clive Randall, Associate Professor of Materials Science and Engineering, B.S. (East Anglia), Ph.D. (Essex)

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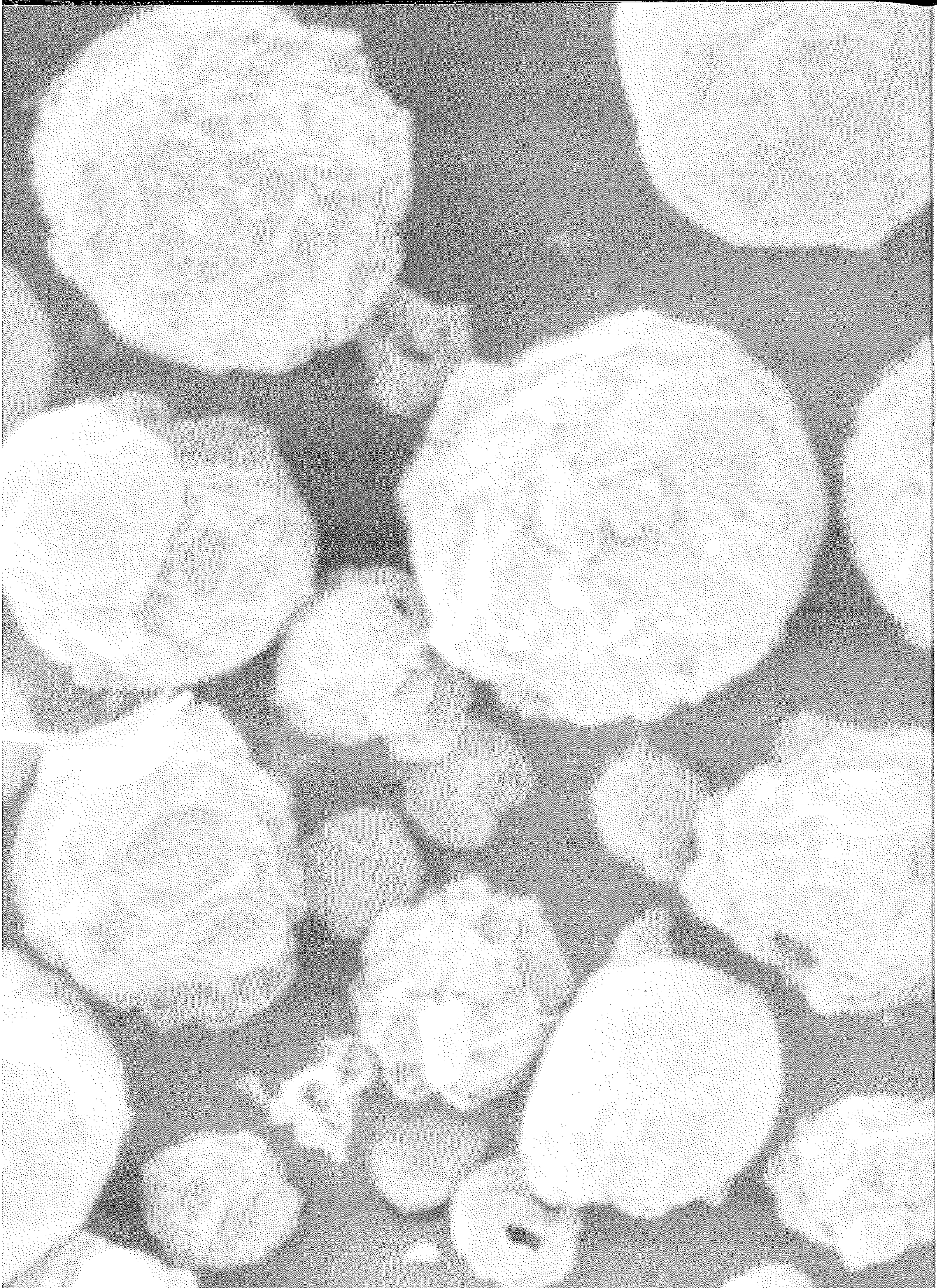
Walter A. Yarbrough, Assistant Professor of Ceramic Science and Engineering, B.S. (Univ. N.C.), Ph.D. (Penn State)



Cenospheres (Ping-Pong ball-shaped spheres) generated by rapidly

Fuel Science (F SC)

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

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 (carbonization, liquefaction, gasification, 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

André L. Boehman, Assistant Professor of Fuel Science, B.S.Me. (Dayton), M.S.Me., Ph.D. (Stanford)

Semih Eser, Assistant Professor of Fuel Science, M.S. (Middle East Tech. Univ., Ankara), Ph.D. (Penn State)

Patrick G. Hatcher, Professor of Fuel Science, B.S. (NC State), M.S. (Miami), Ph.D. (Maryland)

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

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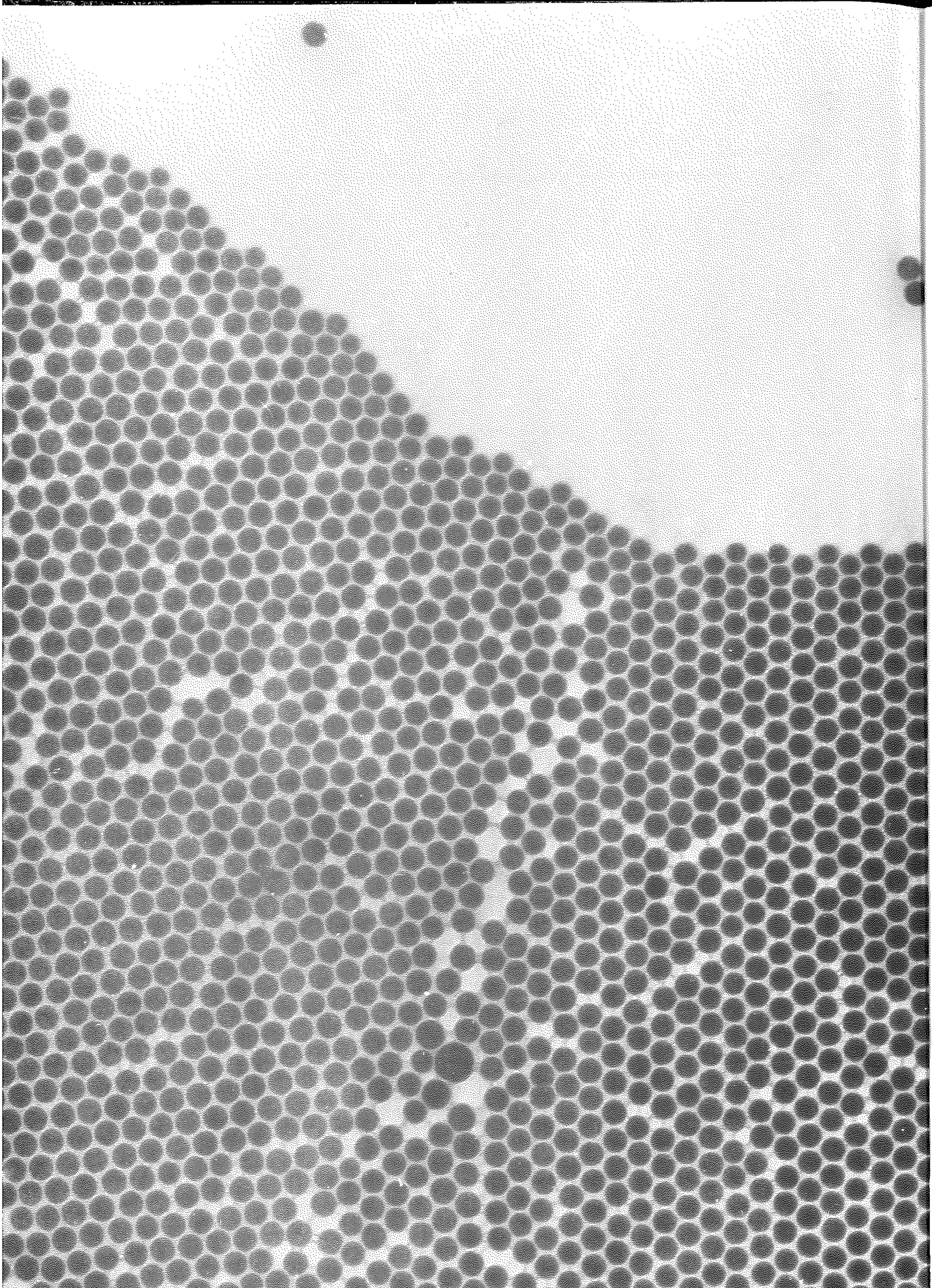

TEM micrograph of SiO_2 particles prepared by hydrolysis of

Metals Science and Engineering (METAL)

DR. K. OSSEO-ASARE, IN CHARGE OF GRADUATE OPTION

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 metal matrix composites, and phase-transformation studies also are extensive.

FACULTY

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Tarasankar DebRoy, Professor of Materials Science and Engineering, B.E. (Burdwan), Ph.D. (Indian Inst. of Science)

John H. Hoke, Professor Emeritus of Metallurgy, D.Eng. (Johns Hopkins)

Paul R. Howell, Professor of Metallurgy, B.A., M.A., Ph.D. (Cambridge)

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Robert W. Lindsay, Professor Emeritus of Metallurgy, B.S. (Tufts), Sc.M. (MIT), Sc.D. (MIT)

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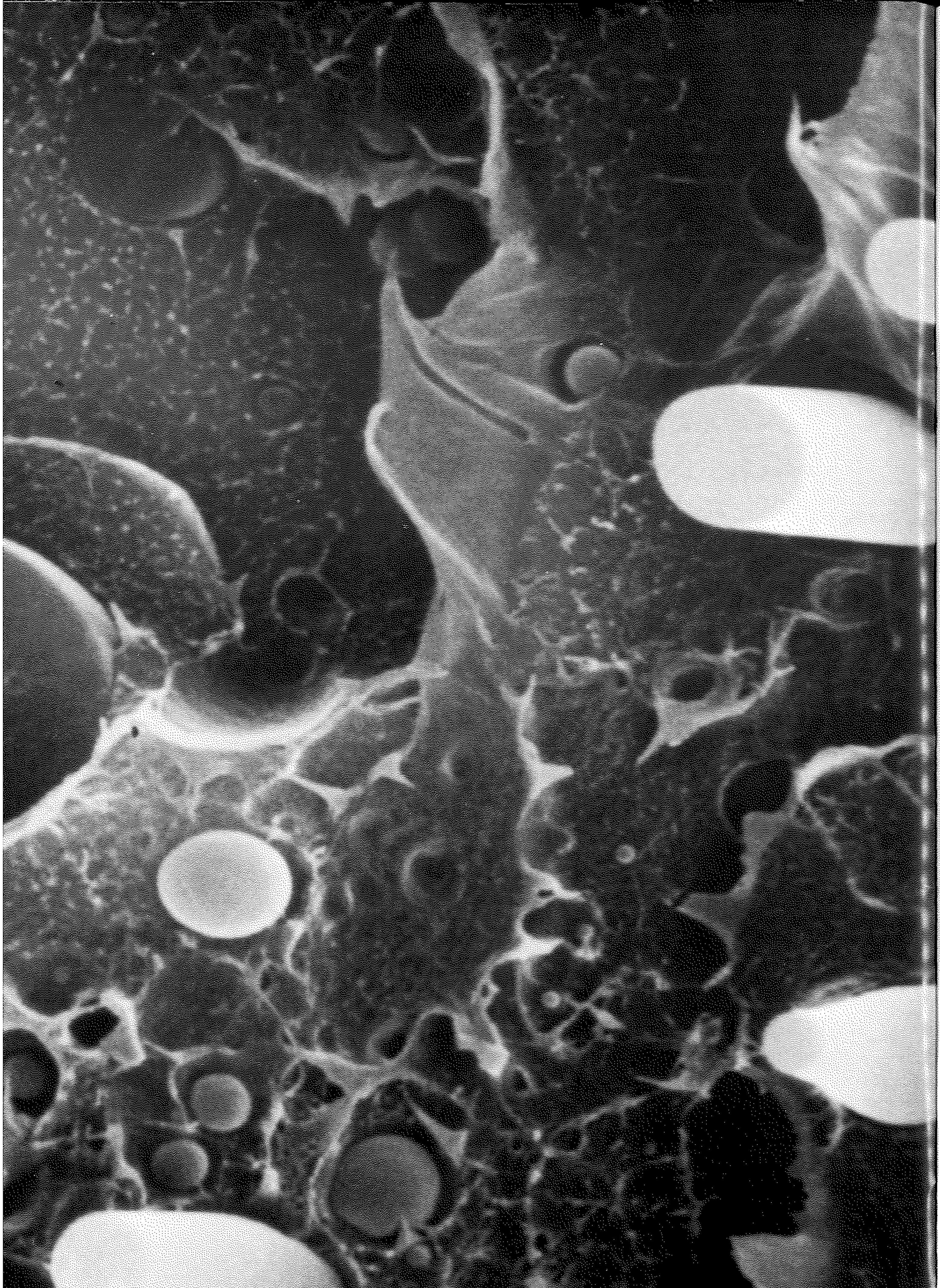
Earle Ryba, Associate Professor of Metallurgy, B.S. (MIT), Ph.D. (Iowa State)

George Simkovich, Professor Emeritus of Metallurgy, B.S., M.S., Ph.D. (Penn State)

Polymer Science (PLMSC)

DR. PAUL C. PAINTER, IN CHARGE OF GRADUATE OPTION



Scanning electron micrograph of a compatibilized blend of nylon and low-density polyethylene (LDPE) depicting the in situ formation

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

David L. Allara, Professor of Materials Science and Chemistry, B.S. (California), Ph.D. (UCLA)

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

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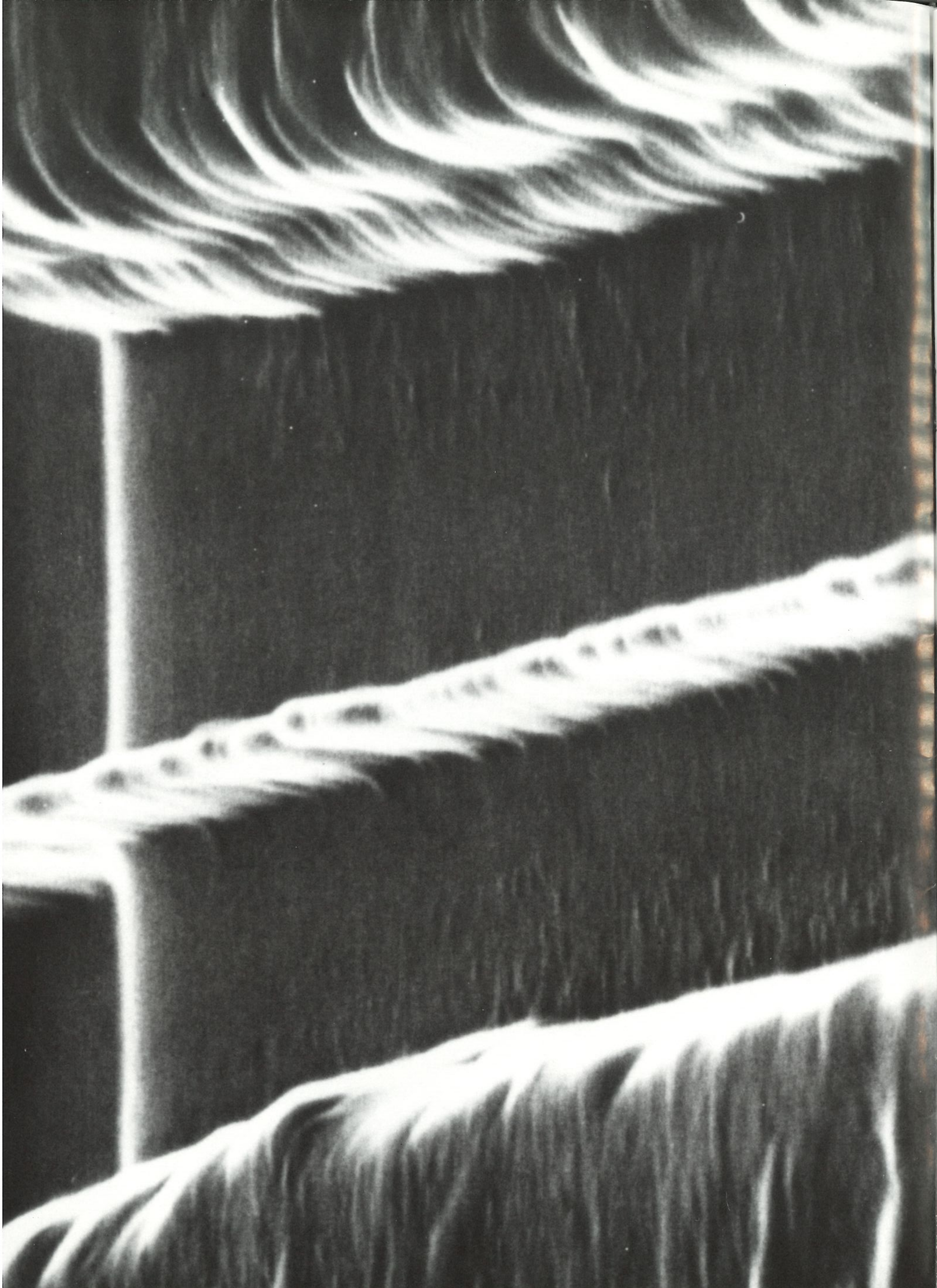

Electronic and Photonic Materials (EPM)

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 other 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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Susan Trolier-McKinstry, Assistant Professor of Materials Science and Engineering, B.S., M.S., Ph.D. (Penn State)

Walter A. Yarbrough, Assistant Professor of Ceramic Science and Engineering, B.S. (Univ. N.C.), Ph.D. (Penn State)

Ultra short gate-length self-aligned GaAs field effect transistor.

)avid L. Allara

Chemistry at Interfaces

: unique molecular and atomic features of interfaces between materials often control ignificantly influence the useful functions of ı synthetic and naturally occurring struc- :s. Examples include the rate and specificity lectrochemical processes, the adhesive ngth and conductivity of thin metal-film :ings on polymer or ceramic substrates in an tronic circuit component, the biological ıpatibility of a synthetic biomedical im- ıt, the efficiency of a semiconductor transis- with a chemically modified interface, and corrosion of a structural metal part induced ts working environment.

[he major objective of Professor Allara's arch program is the development of a fun- ıental understanding of the chemical struc- s and processes that occur at these rfaces. Particular emphasis is placed on in- ıces where one of the adjoining phases is ınic.

\n interface is a complex boundary region can be viewed as a slice of material, often ıin as one or two molecules. Extreme de- ıds are placed on the chemical and struc- l probes needed to study these regions. ra researches both the development of sensi- molecular-structure probes, and the devel- ıent of informative model chemical ctures.

)ne type of model consists of a supported of monolayer dimensions such that all the ecular groups examined will be part of the rface. For example, to learn about the inter- between a polymer and a metal oxide, ra has studied the properties of an absorbed 'mer monolayer on a smooth, planar metal ;trate covered by a thin oxide film. Another lel system of great utility is an organized ıolayer assembly of multifunctional .nosulfur compounds on a gold surface. chment to the gold occurs via a bivalent ır atom. Other groups such as amino, hy- ;yl carboxylate and derived esters, methyl, fluoroalkyl arrange themselves in the inte- or at the ambient interface as dictated by modynamics and molecular structure. An lized top view of alkanethiolate assembly on ı(111) surface is shown in the accompany- figure. These model structures have pro- d details about the molecular basis of the :ing of liquids by an organic surface, the sport of electrons and ions through layers of l groups, and adhesive chemical-bonding ractions in polymer coatings. Other re- :h groups recently have extended this work ıe preparation of biologically active sur- ;, and Allara's group is now examining e structures for use in specific chemical sen-

One of the fascinating aspects of these :ms is the alteration of chemical-reaction hanisms of organic groups because of the "two-dimensional" nature of the assembly. New activity in the research program has been developing additional model structures on technologically important substrates such as glass, carbon, and various semiconductors and recent work has focused on developing new integrated circuit processing methods using monolayers on semiconductors.

Characterization of the above and related structures has been performed primarily by infrared vibrational spectroscopy, optical wavelength ellipsometry, X-ray photoelectron spectroscopy, and electrochemistry. In the case of vibrational spectroscopy, it has been necessary to develop new types of experimental and theoretical approaches in order to provide quantitative characterization of structural features such as surface orientation, group conformations, and intermolecular interactions. Both Fourier-transform and laser techniques have been applied experimentally, while a combination of molecular vibration analysis and classical electromagnetic theory have proved useful for theoretical interpretations. In addition, other promising techniques are continually being evaluated. Of recent interest are scanning tunneling microscopy, quartz crystal microgravimetry, surface plasmon resonance spectroscopy, secondary ion mass spectrometry, forward recoil spectroscopy, and valence band spectroscopy.

Publications

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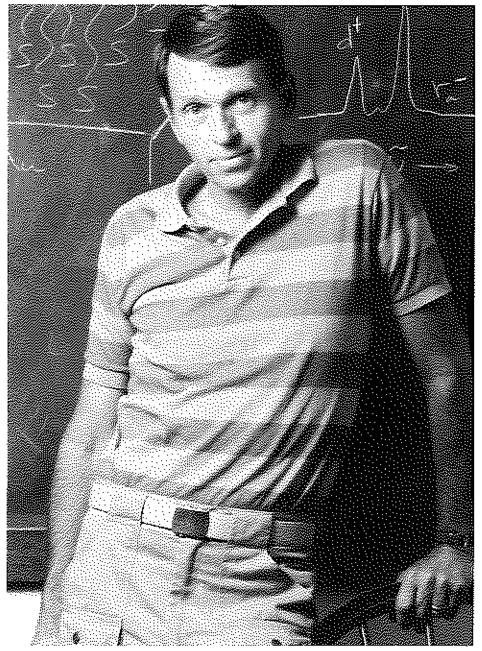

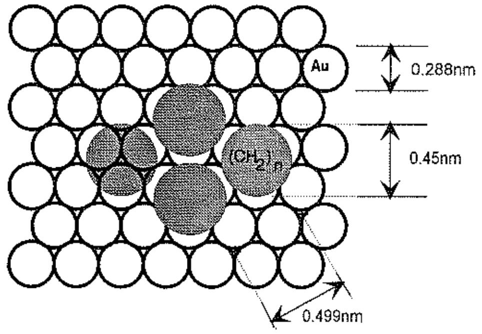

Figure 1. Alkyl chains spaced as next-nearest neighbors on a Au(111) surface.

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Keywords

surface chemistry, chemical kinetics, vibrational spectroscopy, condensed matter interfaces including polymers, surface analysis, materials chemistry

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André L. Boehman

Heat and Mass Transfer in Combustion and Pollution Control Systems

Professor Boehman's research interests involve the study of combustion and pollution control systems for applications ranging from pollutant formation in diesel engines to catalytic pollutant removal from flue gases. These research efforts have included the development of unique experimental facilities for the study of pollution control catalysts, laboratory facilities for measurement and detailed chemical analyses of automobile emissions, numerical models for the behavior of catalytic combustors and pollution control catalysts, and laboratory reactor facilities for pyrolysis studies of aviation fuels.

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, Boehman supervises laboratory facilities for studying pollution control devices and advanced catalysts for use in diverse applications, including diesel oxidation and lean-NO$_x$ catalysts and NO$_x$ abatement systems for industrial coal boilers. This facility consists of a fixed-bed flow reactor, test cells for a single-cylinder diesel engine and a V-8 turbodiesel engine, and instrumentation for sampling gaseous and particulate emissions. The engine laboratory is supplemented by the fuel science analytical chemistry laboratory, which permits detailed chemical analysis of the exhaust composition. New facilities also include flow reactors for thermal stressing of aviation fuels to be used in the development of advanced thermally stable fuels that resist formation of pyrolytic carbon deposits.

Other ongoing research includes the development of numerical models for the transient behavior of natural gas-fired catalytic combustors and the competing reactions over pollution control catalysts. The objective in the catalytic combustion studies is to develop a comprehensive numerical model that includes detailed surface chemistry for multicomponent reactions over an advanced palladium oxide catalyst and detailed homogeneous chemistry for methane combustion. Development of this code will include parallel computing strategies to make use of the computational facilities at Penn State. The numerical predictions will be evaluated by direct comparison with experimental measurements of catalytic combustor performance. The model for pollution control catalysts is being applied to the study of selective NO reduction, wherein the NO reduction reaction competes for the reducing species (ammonia or a hydrocarbon) with the oxidation reaction of the reducing species. This modeling effort has led to formulation of global reaction kinetics for selective NO reduction by hydro-

Publications

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A. L. Boehman, J. W. Simons, S. J. Niksa, and J. G. McCarty. 1997. Dynamic stress behavior in catalytic combustors. *Energy Res. Tech,* in press.

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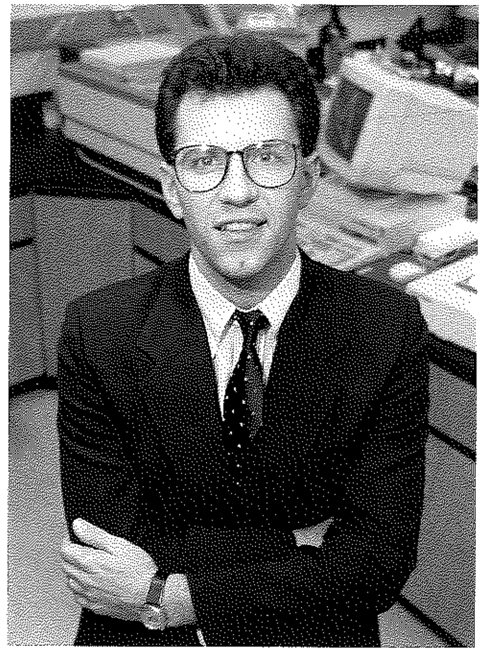

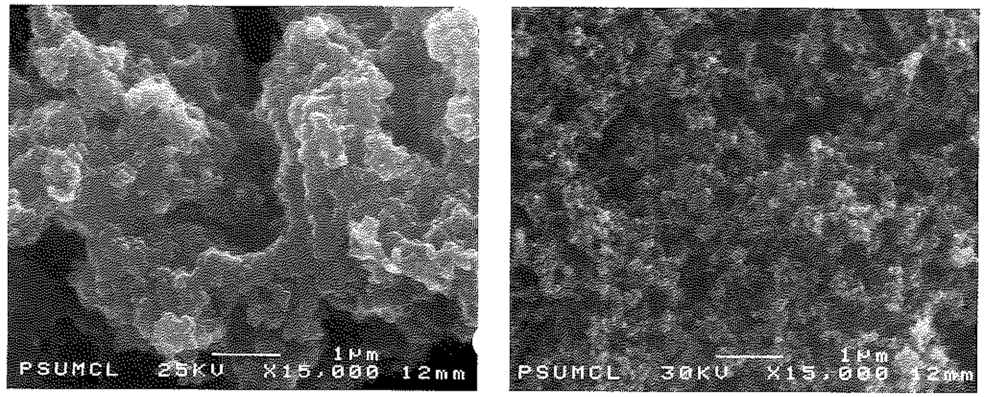

Figure 1. Scanning electron microscope images of diesel particulate matter from (a) a single-cylinder diesel engine and (b) the same engine with ceramic coatings applied to the piston crown, cylinder head, and valves. The thermal barrier coating enhances the oxidation of condensable hydrocarbons that agglomerate with the diesel soot. In figure (b) the particulate matter has a more granular appearance, showing that the soot spherules are not bound together by heavy hydrocarbons.

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Keywords

pollution control, heterogeneous catalysis, combustion systems, NO$_x$, jet fuel, internal combustion engines, heat transfer, mass transfer

’aul W. Brown *Chemical Formation of Ceramics and Composites*

contrast to the conventional sintering pro-
s for inorganic ceramics at temperatures in
:ess of 1,000°C, advanced ceramics and novel
nposites can be formed at low temperature
d atmospheric pressure through controlled
emical reaction. This method of property
velopment has broad applicability to the
mation of both monolithic materials and
amic–matrix composites. Unlike sol–gel re-
ions, chemical reactions produce near net
ipe results so that subsequent high-tempera-
e processing is not required. Fabrication at
: shape, as well as low temperature and pres-
e, involves minimal geometric constraints.
us, composites can be made using combina-
ns of materials that would be precluded if
ocessing were to occur at high temperature
d pressure. For example, ceramic–matrix
nposites combining nontraditional constitu-
s, such as metals or polymers, can now be
ithesized. In addition, precursor phases of
itinuous fibers can be introduced to produce
h-toughness composites, even in composites
it are not fully dense.

As a generic example of a benefit of chemi-
formation, sequential chemical reactions can
used to first form a fibrous phase that is sub-
uently infilled by a matrix phase as the result
a second set of reactions. If the nonmatrix
ase is organic, it can be functionalized to
ifer specific desirable properties to these
nposites. Applications for chemically pro-
ced ceramics and composites range in scope
m the structural to electronic fields. For
ictural application, high toughness can be
iieved; for electronic applications, useful
perties such as chirality can be conferred on
organic constituent to produce piezoelectric,
oelectric, or chromophoric composites.

Dr. Brown’s group has demonstrated the
emical formation of a variety of ceramics and
nposites including the formation of hy-
oxyapatite (HAp) and HAp-collagen compos-
s, of the cristobalite polymorph of aluminum
osphate, and of alkali zirconium phosphates.
\p has been synthesized within a few hours at
ysiological temperatures and under condi-
ns compatible with those in vivo.

Phase pure, porous monoliths of the high-
nperature cristobalite polymorph of $AlPO_4$
ve been synthesized at 130°C, approximately
0°C below the temperature at which
stobalite is in the thermodynamically stable
ase. Phase pure monolithic alkali zirconium
osphate has been prepared at 500°C; mono-
is of the precursor phases have been prepared
ow as 60°C. This later class of ceramics is
iuinely multifunctional and is of interest as a
id state electrolyte, low thermal expansion
terial, and low thermal conductive material.

Publications

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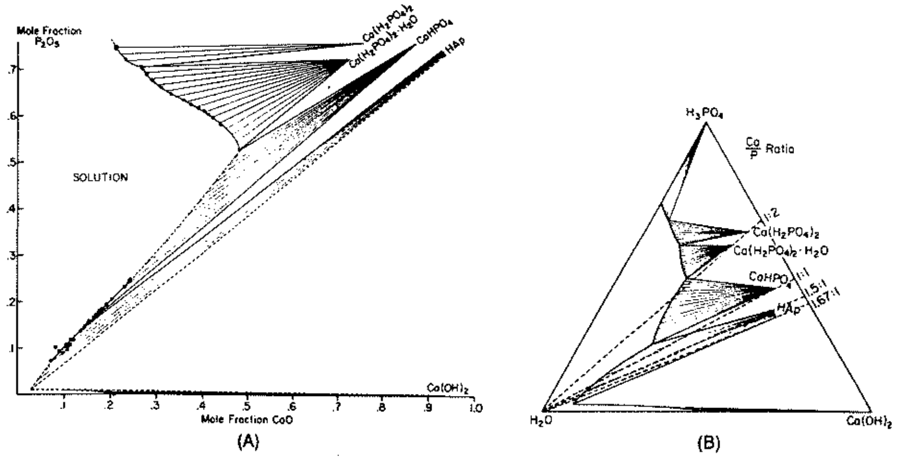
Figure 1. The ternary diagram: CaO-P_2O_5-H_2O at 25°C showing the stability regions of biologically important compositions.



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Keywords

chemical formation of ceramics and composites, bioceramics, biocomposites, multicomponent phase equilibria, low-temperature synthesis

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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 microscope (TEM). Current studies include explorations of segregation and precipitation at ceramic grain boundaries, development of electron holography, active metal brazing of ceramics and ceramic–matrix composites, synthesis of novel complex compounds (dilute ceramics) that are often found as reaction products between ceramics and metallic alloys, and investigation of interface structure and defects in oxide thin films. The first two projects are briefly described here.

The controlled development of anisotropic microstructures in ceramics holds considerable promise, since platelet- 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 platelet (grain at upper left) exhibits an intergranular amorphous phase at the boundary with an adjacent, randomly oriented alumina grain. The crystal lattice planes are imaged directly in both grains. In situ chemical analysis by energy dispersive spectroscopy (EDS) allows us to determine that the amorphous phase (only 1.3 nm in width) is an aluminosilicate containing the intentional dopant titanium. Other grain boundaries are devoid of this phase, and its preferential formation along the basal planes of alumina appears to be closely linked to the development of the anisotropic microstructure.

In other 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 wavefront 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 interferogram, the phase and amplitude components of the electron wave can be separated, providing a wealth of information on three-dimensional shape, electric fields, chemical variations, and other features.

Publications

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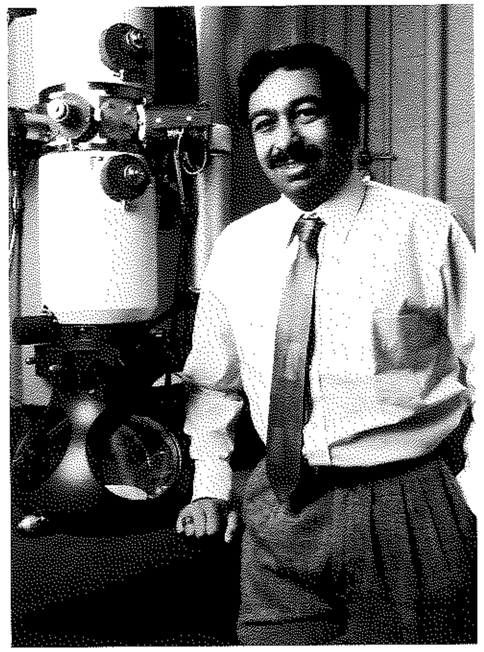

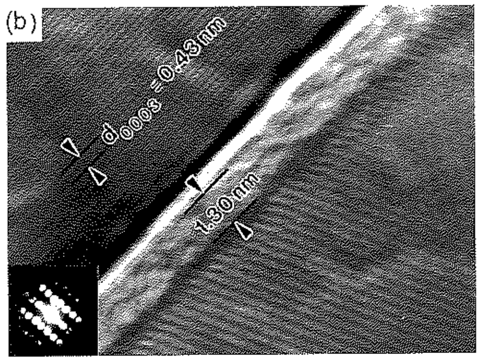

Figure 1. High-resolution TEM micrograph of the (0001) basal plane boundary of a platelet-shaped grain (upper left) in Ti-doped Al_2O_3. The grain at the lower right is oriented randomly. The amorphous phase of ~1.3 nm thickness at the boundary is an aluminosilicate glass that is observed only along basal facets in these samples. Lattice imaging shows the crystal planes within each grain, which clearly demarcate the extent of the amorphous interlayer.

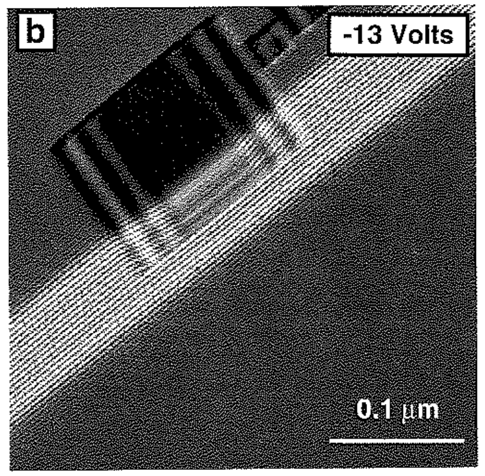

Figure 2. Electron holograph of a fine cubic particle of MgO, viewed along the [210] direction. The high-contrast white fringes across the central portion arise from interference of the object and reference waves; their local intensity variations and displacements allow the separation of the phase and amplitude of the electron wave at any point in the image.

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Keywords

transmission electron microscopy, electron holography, interfaces, grain boundaries, crystal defects, ceramic joining, brazing, thin films

Long-Qing Chen *Computational Materials Science*

l of Dr. Chen's research projects involve the
e of computer workstations and super-
mputers to model and predict the structures
d properties of materials.

Computer simulation and modeling is one
the most rapidly developing and exciting
lds in materials science. Graduate students
rking in this area come from very diverse
ckgrounds including materials science,
amics, metallurgy, physics, chemistry, etc.
mputational models applied in materials
ence are generally categorized according to
ee different spatial length scales: atomic
le, mesoscale, and macroscale. Models in the
mic scale deal with the structures, dynamics,
d physical properties of an assemblage of at-
s, with the number of atoms from a few to
llions. Meso-scale models are concerned with
material's internal microstructure, which is
aracterized by the shape, size, and spatial ar-
gement of phases, domains, and/or grains.
acro-scale models completely ignore the in-
nal atomic- and mesoscale structures of a
terial and describe its behavior using consti-
ive relations and empirical laws based on
ssical continuum theories. Chen's main re-
rch focus is on the mesoscale—in particular,
modeling the temporal and spatial evolution
meso-scale microstructures during
id ⟶ solid phase transformations and dur-
sintering, ferroelectric domain growth,
in growth, and Ostwald ripening, which are
underlying processes for the development of
st of the advanced engineering ceramics and
ys.

Some specific examples of ongoing projects
Chen's group include: (1) evolution of do-
in structures in ferroelectric oxides, driven
the total reduction in the electrostatic en-
y, elastic energy, and domain-wall energy, as
ll as by applied fields; (2) anisotropic grain
wth; (3) coarsening of a solid–liquid two-
ase mixture at high-volume fractions of solid;
microstructural evolution during simulta-
us grain growth and Ostwald ripening in
-phase solids, driven by the reduction in the
al grain boundary and interphase boundary
rgy; (5) kinetics of precipitation of ordered
ermetallics and precipitate coarsening in bi-
y and ternary alloy systems; and (6) control
recipitate morphology and distributions in
-phase alloys by applying an external stress
d. A gallery of microstructures predicted
m their computer simulations are shown in
ure 1 for various processes.

Publications

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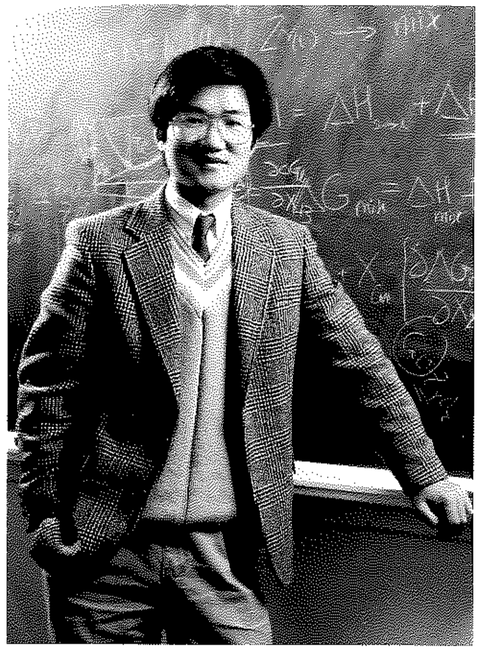

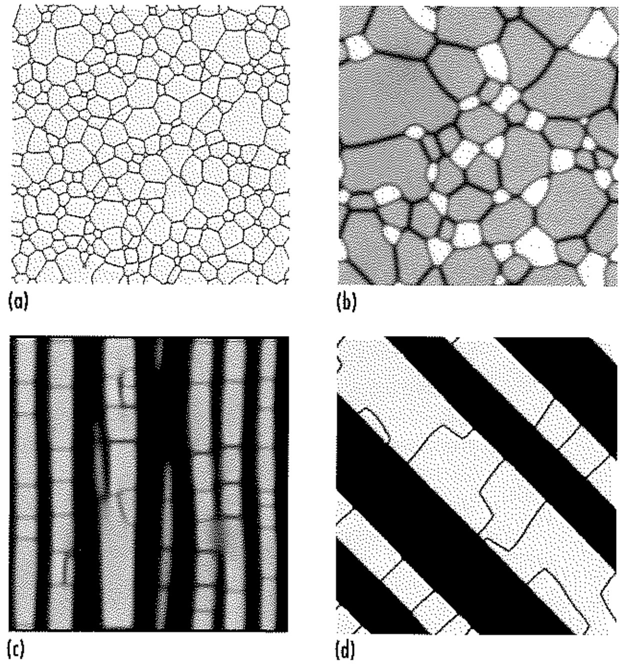

(a) A single-phase polycrystalline grain structure; (b) a two-phase (ZrO_2+Al_2O_3) polycrystalline grain structure; (c) a twin structure formed during a cubic–tetragonal transformation in Y_2O_3-stabilized ZrO_2; and (d) a rafted two-phase (γ+γ') microstructure in a Ni-based superalloy aged under an externally applied stress.

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Keywords
computational materials science, microstructural evolution, phase transformations

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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 polyolefin is a useful method for modifying the chemical and physical properties of polymers, (e.g., adhesiveness, compatibility, and dyeability). 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 intermediacy of borane monomers and polymers. Borane moieties 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 reactional conditions. A broad range of polyolefins, such as PE and PP, with various functional groups (e.g., OH, NH_2, and halides), have been prepared.

The borane-containing polymers have also been used for the preparation 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 hydrophobic and hydrophilic polymeric segments. Several interesting graft polymers consisted of polypropylene, poly (1-octene), and polyisobutylene as the backbones, and several free radical polymers, such as PMMA, PVA, and PAN, 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 polyolefin as the supported materials. The catalyst can be recovered and reused for many reaction cycles. The functionalized and grafted polyolefin copolymers are very effective interfacial materials to improve the compatibility in polyolefin coating, blends, and composites. By using our 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.

Publications

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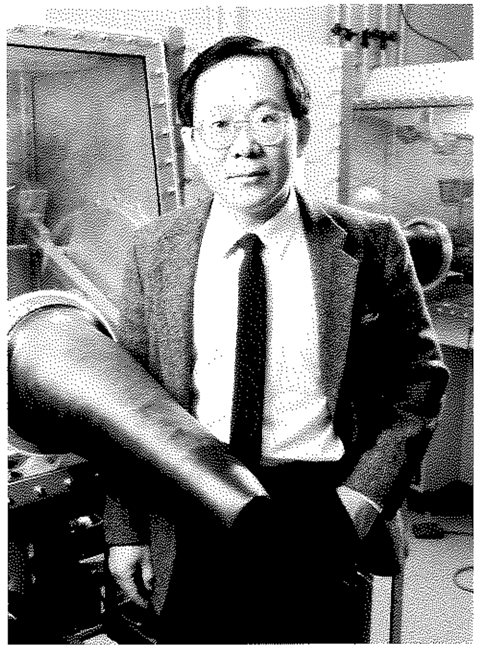
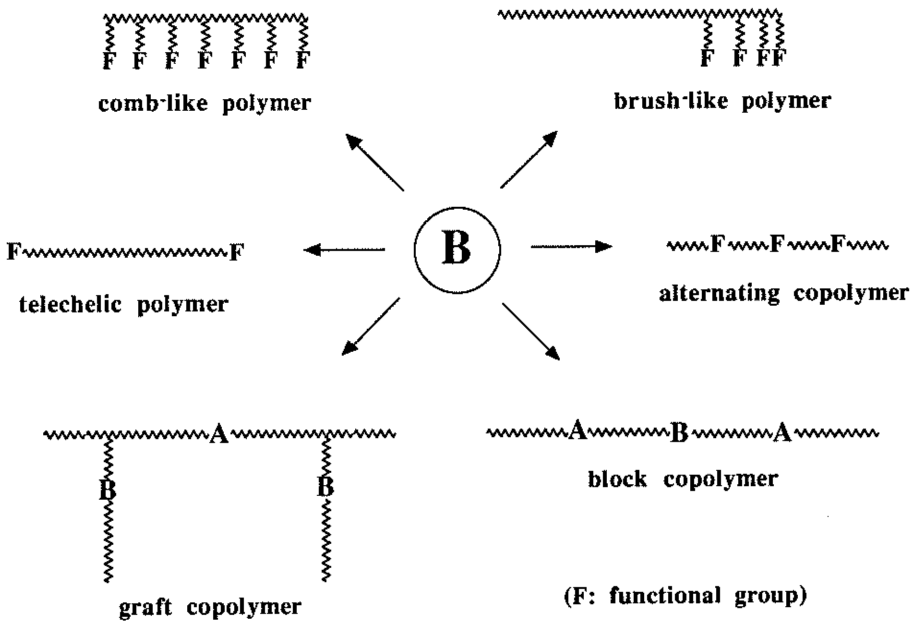


Figure 1. Versatility of borane-containing polymers in functionalization of polymers.



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Keywords
functional polyolefin, 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*

sing rheological techniques to experimentally obe the dynamics of polymer liquids is the rust of Dr. Colby's research program. Simple tions of scaling are used to construct models polymer dynamics, allowing for interpretation the rheology data. Current interests include lyelectrolytes, ionomers, liquid crystalline poly-ers, block copolymers, miscible polymer ends, branched polymers, networks of both arged and uncharged polymers, surfactants, d colloidal suspensions.

In many cases, polymer dynamics are con-lled exclusively by the motion of individual ains. In these cases, on time scales longer than time it takes for molecules to diffuse a dis-nce equal to their size, the material flows like a nple liquid. However, when there is large-scale ucture present in the fluid (such as in liquid stalline polymers or surfactant solutions), coelastic response is evident on time scales ich longer than the molecular diffusion time.

An example of this is shown in Figure 1, ich plots oscillatory shear data for a liquid stalline polymer. In this experiment, the quency ω of mechanical oscillation is varied, as to probe the response of the polymer on ferent time scales. The arrow indicates the quency corresponding to the reciprocal of molecular diffusion time. In its nematic ase (solid curves) the viscoelastic response is uid-like at frequencies smaller than the fre-ency for molecular diffusion (reflected in the t that the loss modulus G″ is dominating the ponse at low frequencies).

In contrast, the smectic phase (open sym-s) is still highly viscoelastic on time scales ich longer than the molecular frequency for lecular diffusion (because the storage modu-G′ is comparable to G″ at low frequencies). e smectic structure apparently gives rise to coelastic response of this polymer on long e scales. We are currently designing experi-nts to explore the relation between structure l properties of similar systems in a systematic ion.

Publications

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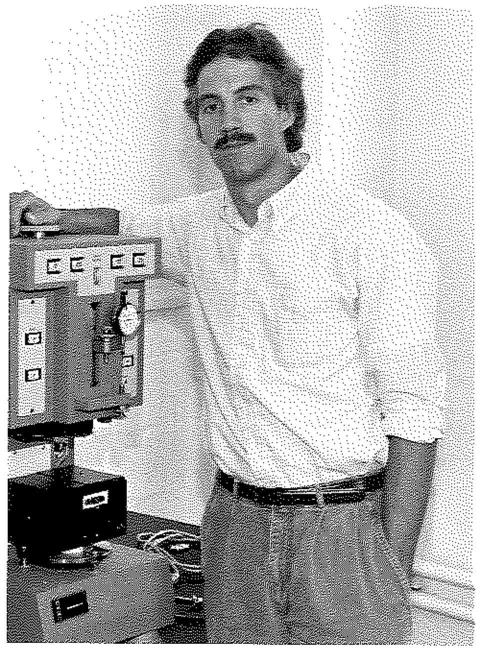
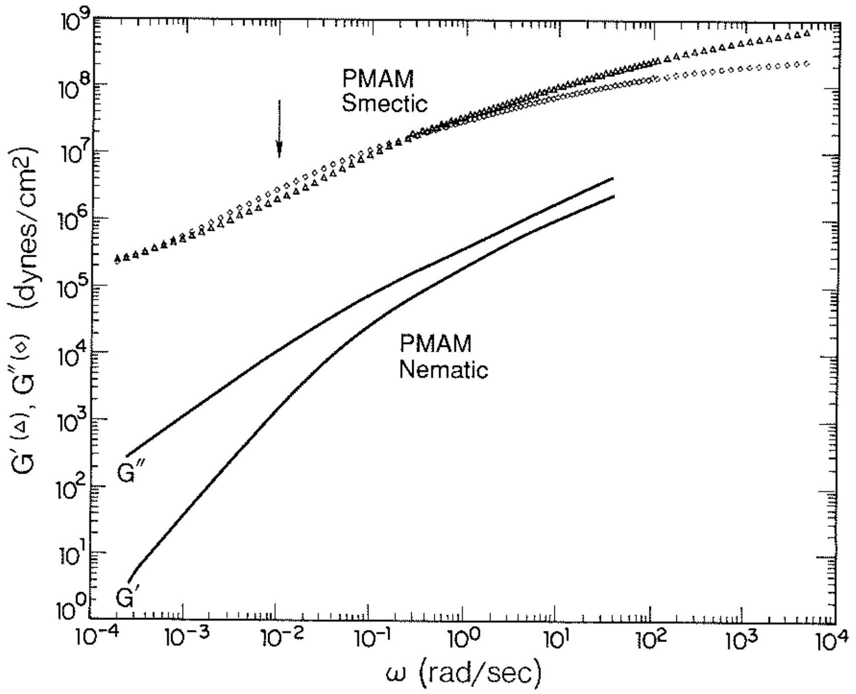


Figure 1. Viscoelastic response of a liquid crystalline polymer in its smectic phase at 84°C (open symbols) and in its nematic phase shifted to 84°C (solid curves). The arrow indicates the reciprocal of the time it takes for the polymer to diffuse a distance equal to its coil size.



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Keywords

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

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Michael M. Coleman *Multicomponent Polymer Systems*

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 (co)polymers 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 copolymers 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. Demands upon the thermal stability of jet fuels are anticipated to become 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 spectroscopies. Using these results as a guide, a number of additives have been identified, most notably benzyl alcohol and 1,4-benzenedimethanol, that retard the formation for carbonaceous solids in Jet A-1 fuels at 425°C.

Publications

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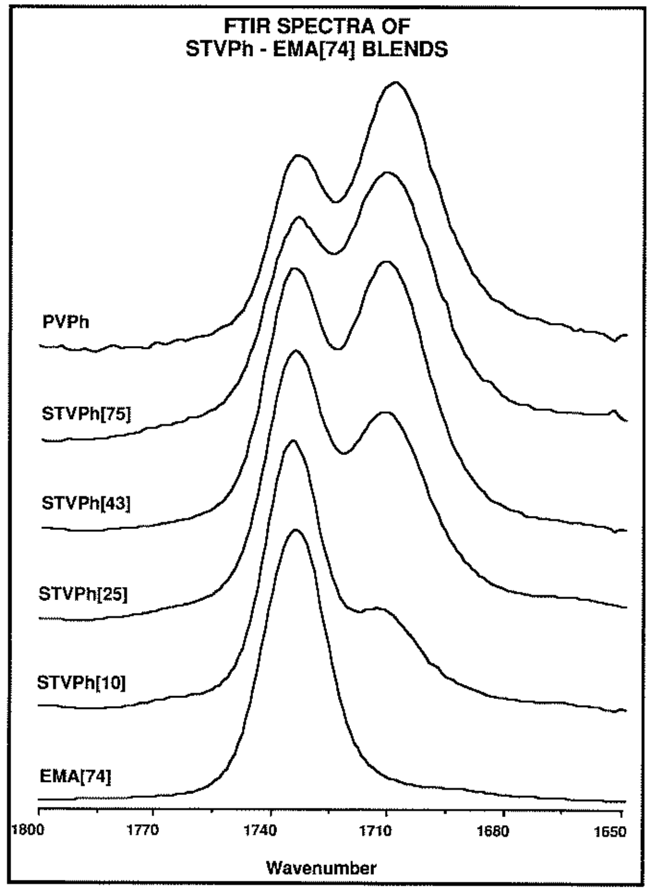
Figure 1. FTIR Spectra of STVPh-EMA[74] Blends



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Keywords

polymer blends, phase behavior, polymer vibrational spectroscopy, hydrogen bonding in polymeric materials, jet fuels stabilization

arasankar DebRoy *Materials Processing and Rate Phenomena*

ıe main focus of Dr. DebRoy's research in-
lves fusion welding processes. His research
olves use of an array of sophisticated modern
perimental tools and physical and math-
atical simulation techniques. Starting with
modeling of heat transfer, flow of liquid
tal, and loss of important alloying elements
ring various fusion welding processes, their
al is to understand how the composition and
ucture of the welded alloys can be controlled.

Recent research by DebRoy and co-workers
fluid flow and heat transfer has led to a
antitative basis for the prevention of variable
netration, which is a major problem in the
lding of steels. Mathematical modeling work
s also led to better understanding of the evo-
ion of weld metal geometry and structure.
ıe nature and amount of various phases and
lusions in the weld metal affect its proper-
s. The group has developed a physical model-
technique to study the partitioning of
drogen, nitrogen, and oxygen between the
ld metal and its plasma environment. The
esence of oxygen, nitrogen, and hydrogen
ects weld metal properties. DebRoy and his
dents have proposed a theoretical basis for
derstanding alloying element vaporization
m the weld pool. They have also developed a
w way of monitoring vapors emitted from
weld pool by light emission studies during
lding. The work is important for weld metal
mposition control and for enhancing envi-
nmental safety during fusion welding.

DebRoy and his co-workers are contributing
the knowledge base that will transform weld-
from an empirical art to an engineering
ence. The importance of this research can be
preciated by the fact that welding is utilized
more than 50 percent of the industrial, com-
ercial, and consumer products that make up
U.S. Gross National Product.

Publications

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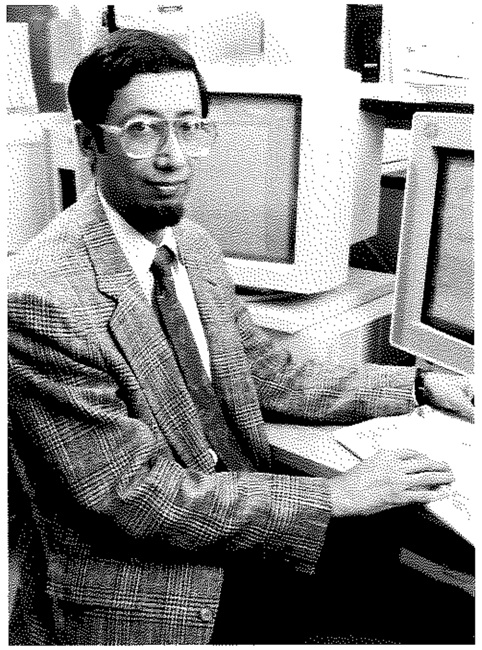

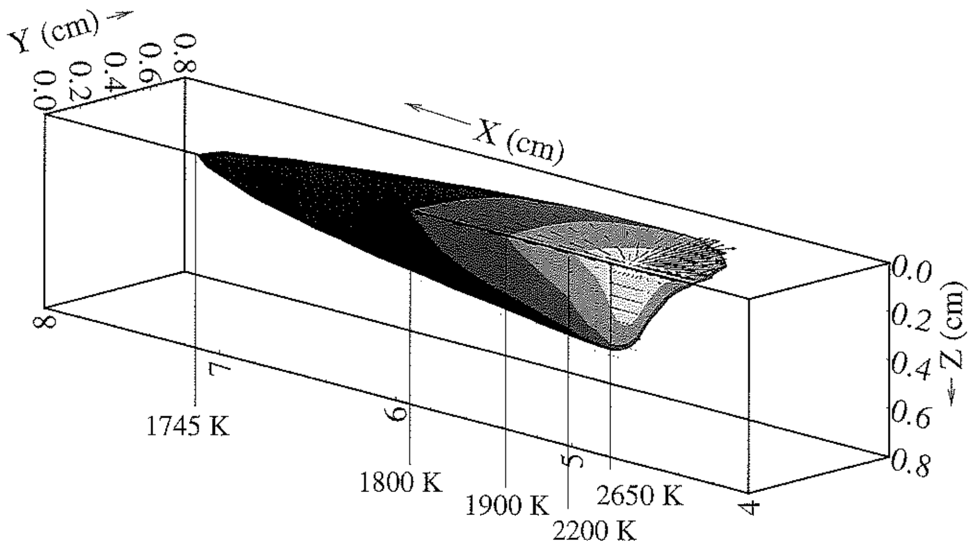

Figure 1. Computed temperature and velocity fields in the weld pool during gas-metal arc welding of a low alloy steel.

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Keywords

plasma processing, welding, laser processing, thin films, numerical calculation of heat transfer and fluid flow, rate phenomena

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Semih Eser *Carbonization, Mesophase Development, Carbon Deposition, Activated Carbon Preparation, Hydroprocessing of Petroleum Residua*

Dr. Semih Eser is carrying out research on carbonization of petroleum feedstocks, microscopic 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 oils produces a premium petroleum coke, called needle coke. Needle cokes are used in the manufacture of graphite electrodes for use in electric-arc furnaces to produce iron and steel from scrap materials. The most significant process that takes place during carbonization in a delayed coker is carbonaceous mesophase development. Figure 1 shows a polarized-light micrograph of a carbonaceous mesophase from a slurry-oil sample, indicating the nucleation of mesophase spheres that coalesce to form anisotropic solid carbon structures. A high degree of anisotropy, as found in needle cokes, is required to manufacture high-performance graphite electrodes.

A major focus of Eser's research program is on seeking a correlation between the molecular composition of the slurry oils and the quality of the resulting cokes. Digital image analysis techniques, developed in the doctoral research program of Ms. G. Qiao, are used to quantify the optical texture of petroleum cokes as a measure of coke quality. A combination of gas chromatography–mass spectrometry (GC/MS), used by Ms. Rose M. Filley in her master's thesis work, and high-performance liquid chromatography with a photodiode array detector (HPLC/PDAD), performed by Ms. Saraswathi R. Kondam, is used for molecular analysis of coker feedstocks. Correlations between molecular composition of feedstocks and the resulting coke texture provide prediction and control of coke quality in industrial coking operations.

Solid carbon deposition on metal and carbon surfaces and thermal degradation of hydrocarbons under supercritical conditions are important concerns for the development of advanced thermally stable jet fuels. Recent experiments conducted by Mr. Jun Li for his doctoral thesis research have shown that some metal surfaces catalyze carbon deposition under conditions similar to those expected in advanced aircraft. Mr. Philip Chang's doctoral research is concerned with the effects of carbon surfaces on carbon deposition from pyrolysis of hydrocarbons. Doctoral research recently completed by Dr. Jian Yu has shown that supercritical conditions affect the thermal degradation mechanisms of hydrocarbons.

In another context with supercritical conditions, Dr. Eser and Dr. Q. F. Zha have shown that polyaromatic hydrocarbons, such as those found in petroleum-heavy residua, can be more

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

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

Publications

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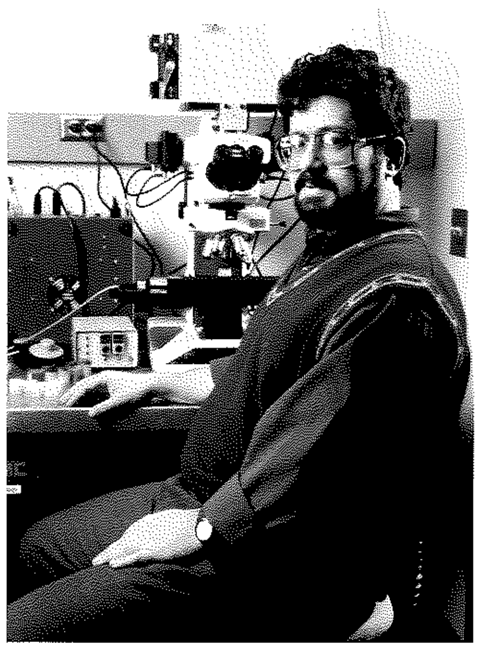

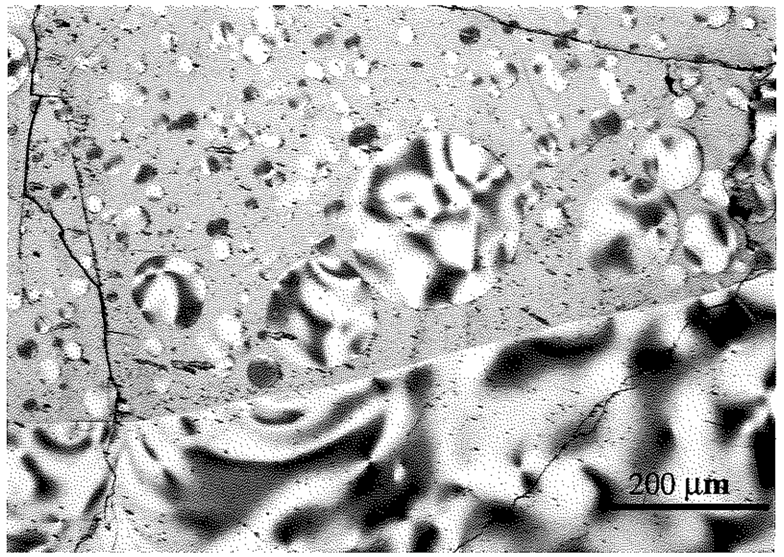

Figure 1. Polarized-light micrograph of a solid produced by carbonization of a decant oil, indicating the mesophase spheres and their coalescence to form anisotropic structures.

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Keywords

carbonization, mesophase, activated carbon, carbon deposition, hydroprocessing of petroleum residua

avid J. Green

Mechanical Behavior of Brittle Materials

amic materials are usually brittle, breaking catastrophic manner. Indeed, this behavior n limits the use of ceramics in both struc- l and nonstructural applications. The low ount of energy involved in breaking these erials is a result of their low toughness. In nt years, however, various mechanisms have n identified for increasing the fracture resis- ce (toughness) of these brittle materials. For mple, improvements in fracture resistance e involved the addition of particles, plate- , whiskers, or fibers to a material. This type pproach has been very successful and, in ne material systems, increases in toughness an order of magnitude have been obtained. ll these developments, the use of a materi- science approach has been a critical philoso- in making the advances. The materials- nce approach emphasizes the relationships ween processing, structure, and mechanical avior as a way to understand a material, and dentify processes for improving its proper-

The physical structure of importance to a ticular mechanical property may occur at ious scale levels. For example, in composites s often the features in the microstructure of a terial that are at the key level for controlling cture resistance. In laminated materials, it y be the macrostructure of the material that critical. The goal of this approach in materi- science is to be able to design structures so t one can obtain a targeted set of properties. r efficient structures, in terms of their weight, nay also be important to control the density the material. In some cases, this is accom- shed by introducing porosity into a material. e overall scientific process is akin to engi- ering design but occurs at all scale levels thin a material.

For the fracture behavior of ceramics, it has ly recently been appreciated that the fracture sistance may depend on the size of the crack at leads to failure. Clearly, this interest has cussed on situations in which this fracture sistance increases with increasing crack size, aking the progress of the crack more difficult it grows. Indeed, it would be of particular terest to be able to control this fracture resis- nce at various scale levels. For example, it has en shown that residual stresses could be in- oduced into a material in such a way that ack growth is stabilized, strength is increased, d the strength variability is reduced. Such fects could be obtained from graded and lay- ed material structures. The research areas be- g investigated by Green are centered on the acture behavior of ceramics. These areas in- ude research on toughening mechanisms, de- gn of microstructures (for introducing crack ability and crack arrest into brittle materials), ilure analysis, and techniques for improving

Publications

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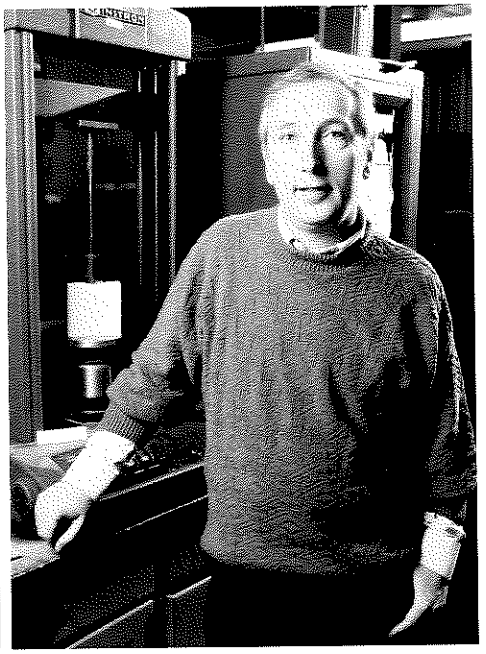
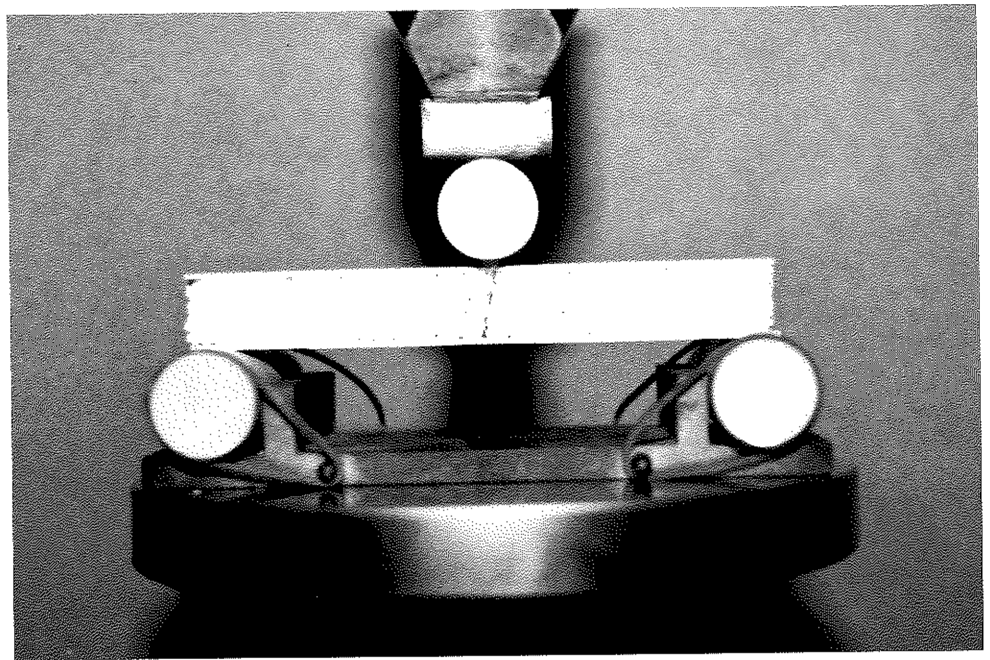


Figure 1. Three-point loading of a ceramic sandwich structure, consisting of a porous cellular core and dense faces. The failure began in the core, but was arrested by the surface layers.



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Keywords

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

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Ian R. Harrison

TREF and PE/LCP Blends

The essence of materials science is structure–property–processing relationships. How do you process materials so they have the necessary structure to produce required properties? Polyolefins 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. Modest changes in chemical structure and processing produce material properties as diverse as foam cushions, bulletproof fabrics, garbage bags, insulated cable, food wrap, and medical devices. Dr. Harrison's work has centered on understanding and developing PE-based materials.

For any polymer, there is a range of properties that it could 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–property relationships and polymer blending are outlined below.

Many polyolefins are made by copolymerizing ethylene with other 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. Both the average and distribution compositions determine properties. In the case of PE copolymers, changes in composition change the ease with which the polymer molecules can crystallize. This property allows us to determine composition distribution. The technique, termed TREF (temperature rising elution fractionation), has been developed at Penn State to a commercial level, and its optimization continues.

Mixing PE with other polymers often produces materials with poor properties. PE, like many other polymers, doesn't like to mix; it's 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 an in situ fiber-reinforced material. With only 10 percent LCP, this composite's stiffness can be made to be five times that of PE; and with additional treatment, its strength is nearly six times that of PE. These unusual composites are being evaluated for a number of applications, and further work is designed to understand and control fiber orientation in this new class of materials.

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

Publications

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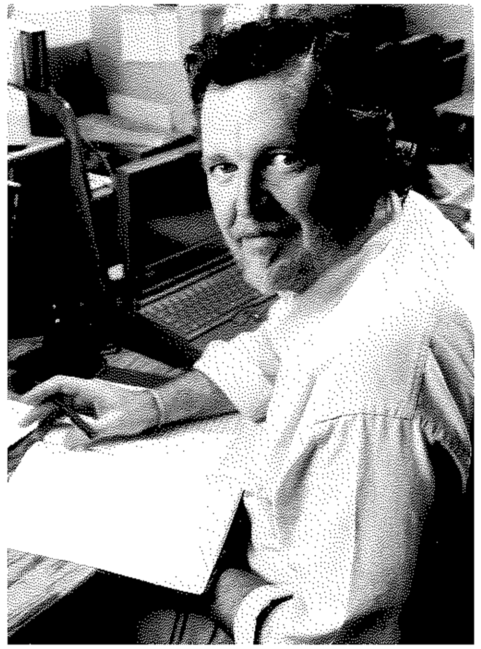

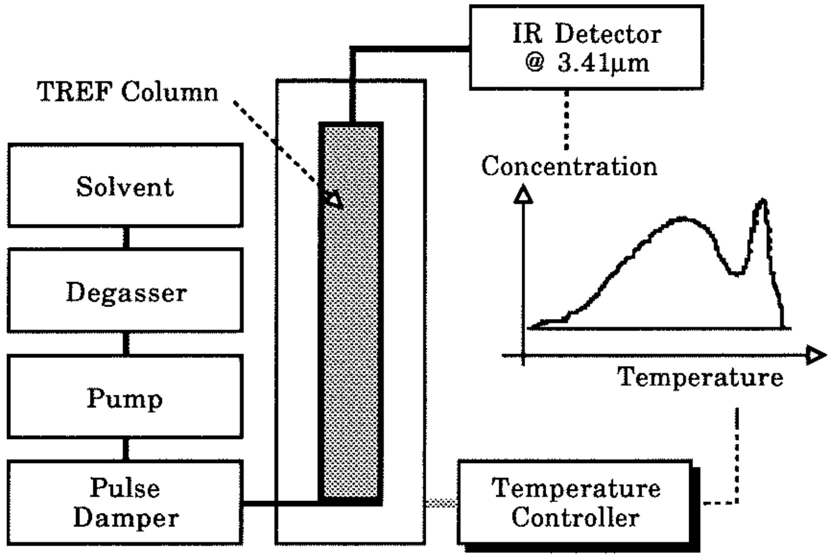

Figure 1. Scematic of TREF apparatus.

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Keywords

structure–property–processing relationships in polymers, TREF, mechanical properties, elongational rheology

atrick G. Hatcher

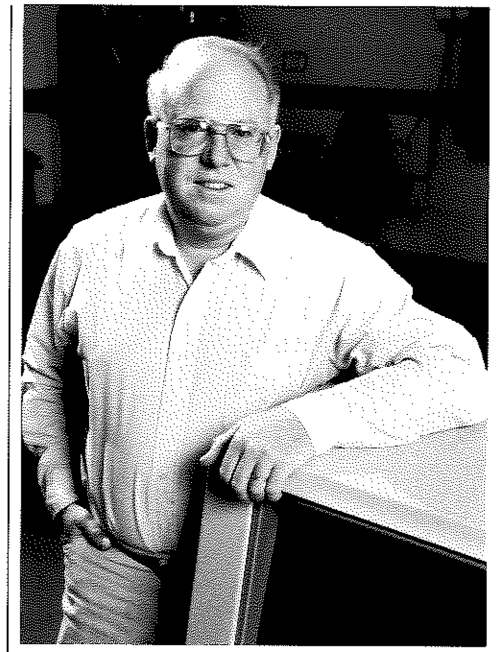
Environmental Chemistry and Geochemistry

ofessor Hatcher and his co-workers are in-
lved in numerous studies in the area of envi-
nmental chemistry and geochemistry,
ecifically emphasizing the origin and chemi-
l transformations of plant-derived biopoly-
ers in soils, peats, coals, marine sediments,
d oceanic waters. A particular focus of recent
terest is in the development of a chemical
iderstanding of the three-dimensional struc-
re of lignin, a large component of terrestrial
ants, and of the transformation of this mate-
l to humic substances in soils and sediments
d, eventually, to coal. Modeling of presumed
uctures of lignin in three-dimensional space
s provided new suggestions that lignin may
ve a helical structure as depicted below (Fig-
e 1). Studies performed in collaboration with
ofessor Mueller's group in the chemistry de-
rtment seek to provide experimental evidence
this structure and involve stereoselective and
giospecific synthesis of ^{13}C-labeled polymers
d use of solid-state ^{13}C NMR techniques to
ablish distance information. Studies with Dr.
inard's group (chemistry) involve isolation
d structural characterization of lignin dimers
d oligomers by a new, jointly developed tech-
que of thermochemolysis with tetramethyl-
monium hydroxide.

This technique is also being applied to the
aracterization of lignin-derived components
d other natural plant-derived biopolymers in
tural systems such as soils, peats, coals, ma-
e sediments, and waters. One application of
rticular importance from the perspective of
global warming issue relates to using this
thod for assessing the transport of terrestrial
d aquatic material to the world's oceans and
sedimentary systems. The timescale of car-
n cycling on Earth depends greatly on the
ount of carbon that is transported to and
ried in these environments, and assessing the
ure and contribution of these biopolymers
not been easy. The above technique will
vide direct measurements of the contribu-
n of refractory biopolymers to sequestered
bon in the global carbon cycle.

Another important area of research in the
tcher group deals with the biogeochemical
nsformation of pollutants such as chlorinated
enols (from herbicides) and polycyclic aro-
tic hydrocarbons (PAHs) from oil contami-
ion. Using a technique developed in the
tcher laboratories involving a site-specific
-labeling/NMR approach, the first direct
dence for covalent binding of pollutants to
humic materials was obtained. Current
rk on the transformation of ^{13}C-labeled
Hs is discovering new chemical pathways for
environmental degradation of these toxic
stances in sediments and soils.

Although the mainstay of the group is appli-
ion of a variety of complex gas chromatogra-
/mass spectrometry and ^{13}C NMR spectroscopy to the study of environmental problems, other research areas involving use of the equipment housed in the Hatcher laboratories include nuclear magnetic resonance imaging of coal to examine dimensionally related changes during solvent swelling, ^{129}Xe NMR of coal and microporous solids to ascertain average pore dimensions and pore morphology, solid-state ^{15}N NMR of coal and natural biopolymers, and kinetic studies of the thermal degradation of petroleum and coal-based fuels.



Publications

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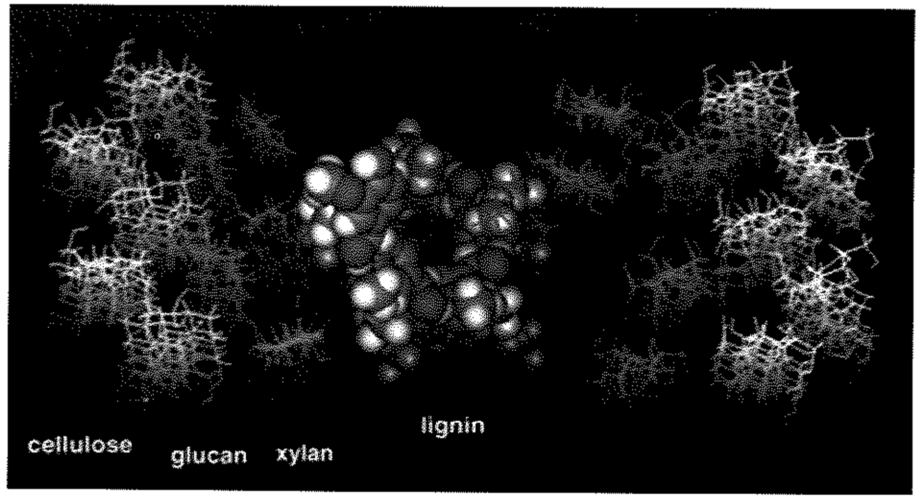

Figure 1. Three-dimensional model depicting ligno-cellulosic complexes in wood.

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Keywords

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

John R. Hellmann

Development of Materials with Tailored Properties

Professor Hellmann's research interests focus on the development of new materials and complementary materials design methodologies for their application as structural and thermal members in high-performance applications. These research efforts cover the range from monolithic to composite ceramic and intermetallic materials. Effects of microstructure on thermal, mechanical, elastic, and optical properties of materials are of central interest in his studies.

Recent studies in Professor Hellmann's laboratory address tailoring of interfacial bonds in model ceramic-fiber-reinforced ceramic-, metal-, and intermetallic-matrix composites to elucidate the key mechanisms that contribute to enhanced high-temperature fracture toughness and creep resistance. His research team's development of novel fabrication methods for such materials is unique, and opens a myriad of possibilities for producing advanced ceramic-composite materials such as high-temperature structural components for the automotive, aerospace, and industrial-heating-systems manufacturing industries. Current efforts are concentrating on the selection and application of fiber coatings to achieve the levels of interfacial bonding and thermoelastic stress relief required for high fracture toughness and high-temperature strength.

A parallel activity in Professor Hellmann's laboratory focuses on establishing test and analysis methods for predicting, and experimentally verifying, physical properties such as thermal conductivity, thermal expansion, heat capacity, optical emissivity, elastic moduli, and interfacial shear strength of ceramic composite materials with tailored microstructural characteristics. His research team has combined finite-element analysis with experimental verification of interfacial shear behavior to assess the relative contributions of thermoelastic stress and applied mechanical stress 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 in his laboratory to developing test methods for interrogating 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 corroborated the applicability of the test-and-analysis methodologies developed. Resulting materials modifications and process improvements will instill systems- and component designers with confidence in advanced materials for high-temperature industrial, aerospace, and automotive applications.

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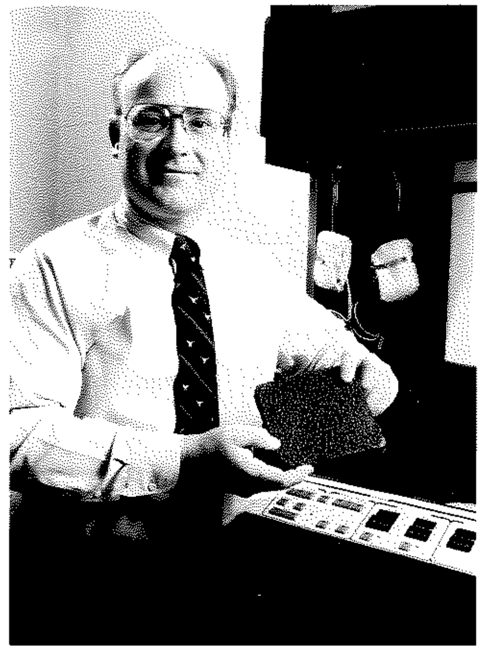

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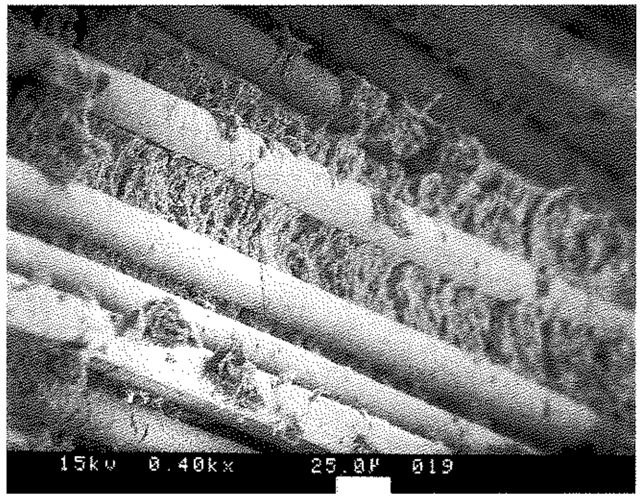

Figure 1. Longitudinal section of an alumina-fiber-reinforced polycrystalline alumina composite made by infiltration techniques developed in Hellmann's laboratory.

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Keywords

ceramics, intermetallics, composites, interfaces, coatings, mechanical properties, thermal properties, processing, microstructure, structure–properties relationships

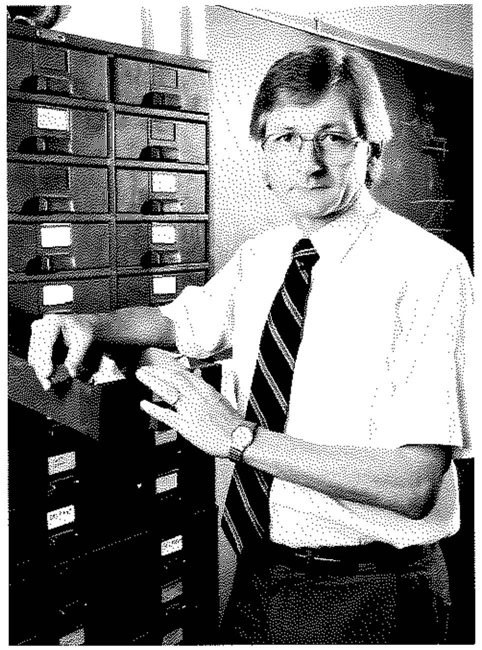
aul R. Howell

Phase Transformations in Metals and Alloys

ofessor Howell is concerned with microstruc-
ral development in metals and alloys. His
rrent research interests include the eutectoid
action in steels and bronzes, phase transfor-
ations in Al-Li/Silicon Carbide composites,
d laser welding of Al-Li alloys, bronzes, and
w carbon steels.

The eutectoid reaction in steels has been of
terest to scientists for many decades. How-
er, the magnetic nature of low-alloy steels
akes them difficult to examine using the
ansmission electron microscope (TEM).
ence, Howell is now examining the eutectoid
action in a class of materials called *nickel-*
uminum bronzed (NAB) materials. These ma-
rials mimic steels in virtually all respects
cluding a martensitic reaction during con-
nuous cooling. Howell and his graduate stu-
ents have shown that the proeutectoid
pper-rich phase is always responsible for initi-
ing the eutectoid reaction, by replacement of
e high-temperature, body-centered cubic
hase with an intimate mixture of the copper-
ch phase and an aluminum-rich intermetallic
hase. A mechanism for the development of the
tectoidal mixture, based on a model for the
rmation of a phenomenologically similar dis-
ntinuous reaction, has been proposed.

Howell has also devised a mechanism for the
rmation of solid-state dendrites of an iron-
ch intermetallic phase in these bronzes and is
reparing a major review on the eutectoid reac-
on in steels.



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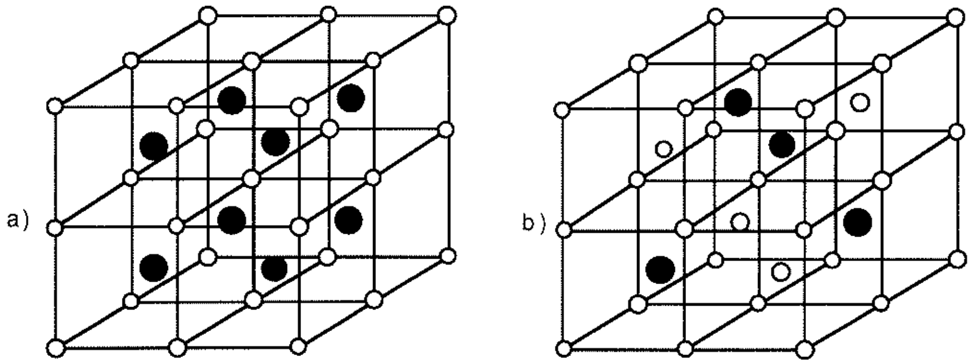
Figures 1a and b. Representation of the crystal structures of two intermediate phases in the nickel-aluminum bronze system.



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Keywords
phase transformations, transmission electron microscopy, steels, aluminum, bronzes, welding

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Donald A. Koss

Ductile Fracture and Failure Criteria of Steels

The performance of load-bearing structures under complex loading conditions ultimately 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' response under the imposed loading conditions. Such predictions are complicated by the fact that most engineering structures are typically subjected to multiaxial stress states that are spatially nonuniform and often contain weldments, resulting in material properties that, in turn, vary spatially.

Using Navy HY and HSLA steels as model systems, Dr. Koss's research program examines the multiaxial failure criteria and ductile fracture mechanisms characteristic of steel 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 micromechanisms 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 contains several components: an experimental study to determine failure conditions and identify the underlying failure mechanisms, a computational modeling study to address the "void-sheet" mechanism of ductile fracture, and an experimental modeling effort to identify void interactions during fracture.

Publications

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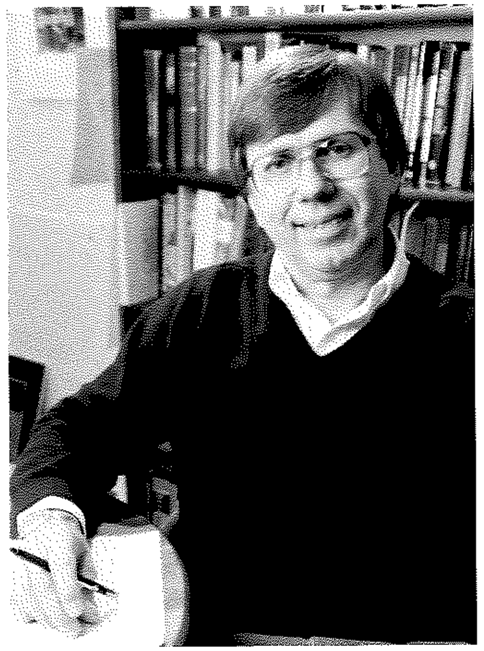

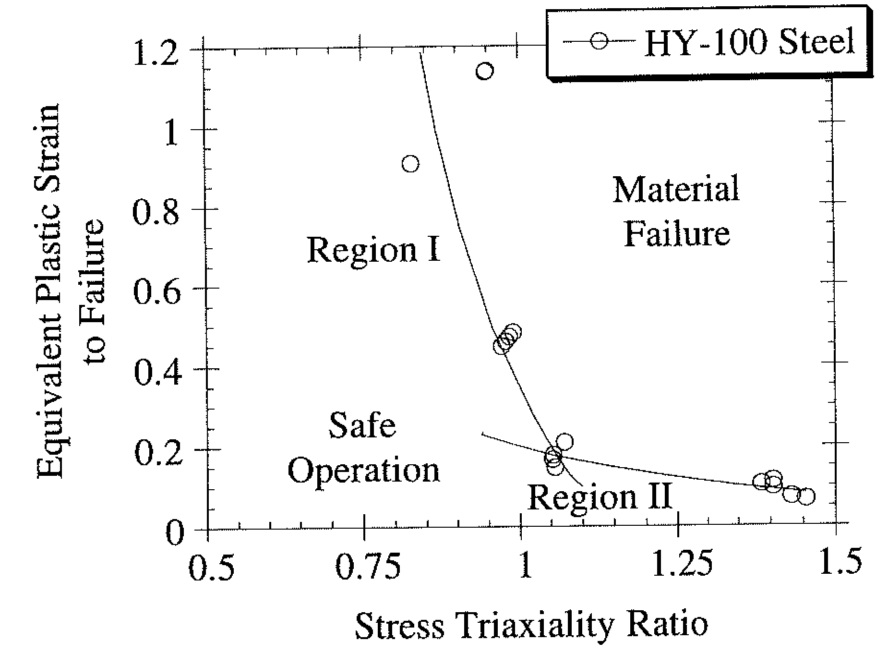

Figure 1. A failure limit diagram indicating failure strains as a function of multiaxial stresses for HY-100 steel.

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

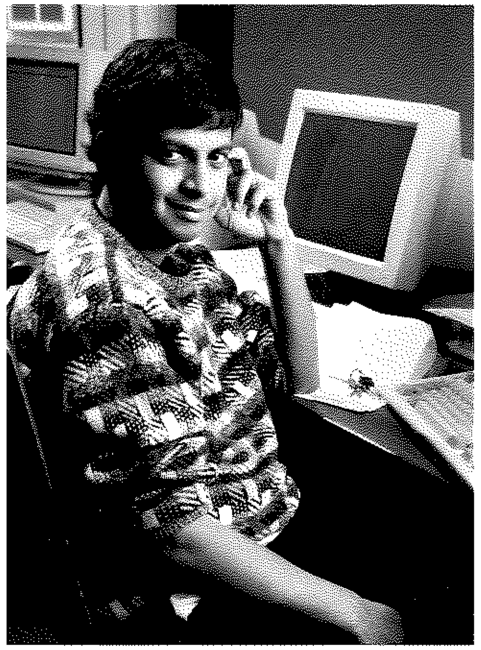
anat K. Kumar

Thermodynamics of Complex Condensed Phase Systems, Polymers at Surfaces and Interfaces, Glass Transition Phenomena, Dynamics of Macromolecular Liquids

: fundamental understanding of the
:mophysical properties of complex con-
sed phase systems, such as polymer mixtures
 polymer–clay composite materials, are criti-
to their use in applications. However, their
:modynamic modeling to date is understood
ost exclusively on the basis of the fifty-year-
 mean-field Flory lattice model. The goal of
 aspect of my research is to utilize computer
ulations on carefully designed model sys-
is to understand the thermodynamics of
ymer systems and their mixtures. Compari-
 of these data to experiments (performed in-
ise and by others) allows for a direct
dation of these ideas. These data will also be
:ctly employed in developing new theories
: can provide an increasingly improved de-
ption of the physical properties of this im-
tant class of materials.

In related work, we are interested in the be-
ior of polymer materials near surfaces and at
:rfaces. We are strongly motivated by prob-
s relevant to applications: in particular,
ting technologies and thin film displays. In
 case of coating technology, the issue of rel-
ace is the phase behavior of thin multicom-
ient polymer coatings and the effect of finite
 on this issue. This question is important
:e the optical quality (such as gloss) and me-
nical strengths of these films are sensitively
:rmined by their phase state. We are cur-
tly conducting an experimental and a theo-
cal program to delineate some of these
es. Specifically, we are in the process of con-
ting pioneering, small-angle neutron scat-
ng experiments to determine phase behavior
hin polymer mixtures. These experiments
 particularly exciting since they are per-
ned on samples with nanoliter volumes and
resent the smallest systems on which scatter-
 experiments have been performed. For thin
ı displays, we are interested in understand-
 the role of uniaxially rubbed polymer films
ırientation layers for the electro-optically
ve component of the display: a small mol-
le liquid crystal. A primarily experimental
gram (supported and performed in collabo-
on with a research group at IBM, Almaden)
: involves grazing incidence X-ray scattering
 near-edge X-ray absorption fine structure
:troscopy is utilized to understand the role
ıuffing in this context. Related to all of these
stions are the fundamentally critical issues
he dynamics of polymer chains in these con-
:d spaces. A combined experimental and
oretical effort has just begun to address the
es in our laboratory.

Another issue of extreme importance from a
cessing standpoint is the dynamics of poly-
: mixtures, especially the role of vitrification.
 are collaborating with Professor Colby of
 department to understand these issues from
ndamental, as well as an applications, standpoint. We conjecture that concentration heterogeneities (or fluctuations) that are present in any mixture have a very strong impact on dynamic properties such as viscosities, diffusion coefficients, etc. Our goal is to study these concentration fluctuations using scattering probes and the resulting dynamics of the system through rheology, dielectric spectroscopy, and neutron spin echo spectroscopy. A theoretical framework is then necessary to capture these results and extend them to a range of practically relevant systems.



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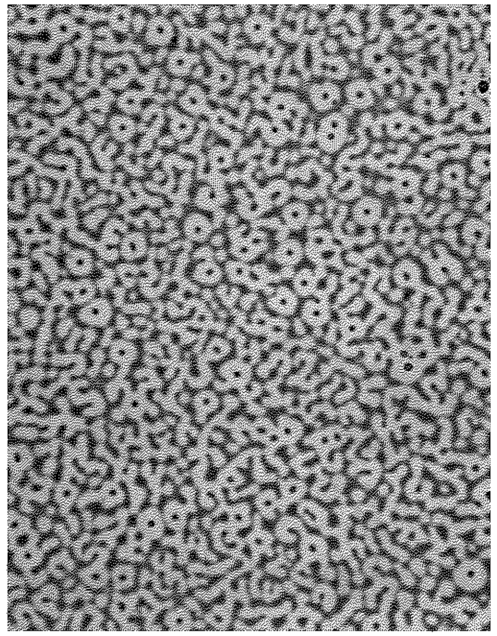

Figure 1. An optical micrograph of a phase separation phenomenon in an ultrathin (50 nm) polymer mixture.

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Keywords

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

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Digby D. Macdonald

Improved Control Over the Operation of Thermal Power Plants

Dr. Digby D. Macdonald is the director of the Center for 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 a 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 director of the physical sciences division of SRI. From 1979 to 1984, he served as a professor of metallurgical engineering and director of the Fontana 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, as chair of the SAB Materials Panel, recently led a study under the New World Vistas program to explore and define the future materials needs of the air force. Dr. Macdonald received the Whitney Award from NACE-International (1992) and the Wagner 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 and the Electrochemical Society. Dr. Macdonald is the author of one book and more than 400 papers in thermodynamics, electrochemistry, corrosion science, chemistry, and materials 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 first field, he has been instrumental in developing the point 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 of the nucleation of localized corrosion damage. He has extended this work to develop "damage function analysis" (DFA), which seeks to provide a deterministic basis for predicting corrosion damage in complex industrial systems. It is for the development and application of this science and technology to nuclear power reactors, and the definition of the electrochemistry of reactor heat transport circuits, that he was selected as the W.B. Lewis Awardee in 1993. He is currently developing DFA as a replacement for the empirically based damage tolerance analysis

complex mechanical systems, including aircraft, power plant coolant circuits, and industrial condensers.

Publications

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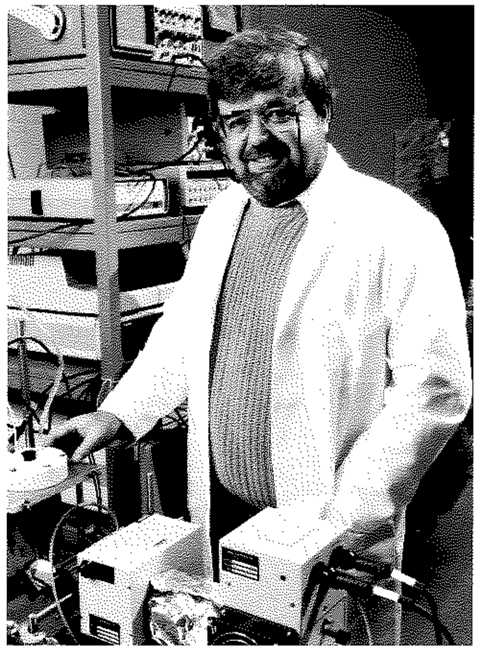

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Keywords

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

Merrilea J. Mayo

Nanocrystalline Materials and High-Temperature Deformation

rofessor Mayo has two main interests: anocrystalline materials and high-temperature eformation. Nanocrystalline materials are etals or ceramics composed of crystals smaller an 100 nm—smaller than the wavelength of isible light! These materials often have very nusual properties; at one time they were seriusly being considered as a new form of matter. ur experience shows us that nanocrystalline etals are ultrahard and wear resistant, ideal for utting tools. Nanocrystalline ceramics, on the ther hand, can actually be ductile at moderate mperatures. This allows them to be formed irectly into parts, or to be used as a kind of lue for joining more conventional ceramics. rom a scientific viewpoint, nanocrystalline aterials are fascinating, since it is the grain oundaries (that is, the interfaces between crysls) and *not* the grains (crystals) themselves at dictate the behavior of the material. In is way, nanocrystalline materials are fundaentally different from normal, larger-grained aterials.

Professor Mayo's laboratory follows the life f a nanocrystalline material from start to finsh: synthesizing ultrafine powders, processing hese powders into bulk form, and testing the inal nanocrystalline product. Development of rocessing protocols is not easy. For instance, a ustomary step in densifying a powder into a olid is to heat the powder. Unfortunately, for anocrystalline powders this heating causes the rains to grow, often to very large sizes. To acomplish densification without grain growth, ayo has explored a number of new processing echniques, such as superplastic sinter-forging, nd has also attempted to understand the role f pores in both the densification and grain rowth processes. Once a viable nanocrystalline aterial is made, it is tested for a number of roperties of interest, such as hardness, fracture oughness, ionic conductivity, diffusion bondng ability, and superplasticity. Superplasticity an extreme form of ductility that manifests tself when fine-grained materials are deformed nder moderate stresses and slow strain rates. his kind of ductility is currently used in aeropace applications to make extremely complex arts in simple, one-step forming operations. Vith nanocrystalline materials, we have the ossibility of further accelerating the forming ates associated with superplasticity to the point vhere mass-market technologies (e.g., the autonobile industry) can take advantage of them.

Publications

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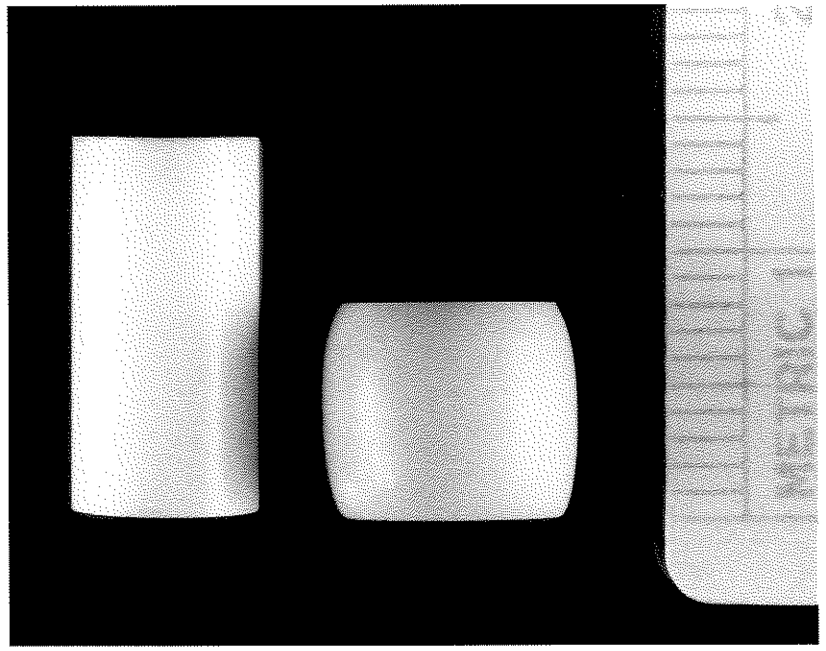
Figure 1. A superplastic ceramic. (a) before deformation, (b) after deformation.



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Keywords

nanocrystalline materials, high-temperature deformation (creep), superplasticity

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Gary L. Messing

Ceramic and Particulate Materials Processing

The fabrication of advanced ceramics with targeted properties requires control over all process stages from powder synthesis through sintering. The complex relations between the myriad processes embraced in ceramic processing is the general focus of Dr. Messing's research program. For example, he and his group have had a sustained 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 chemistries, they have demonstrated unique control of phase development, transformation kinetics, sintering, and microstructure development in alumina, alumina-based ceramics, and mullite. Recent progress in templated 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 thermolysis atmosphere particulate materials and films of mixed metal oxide ceramics, nonoxide-oxide composites, and metals can be prepared.

Publications

Y. Narender and G. L. Messing. 1997. Mechanisms of phase separation in gel-based synthesis of multicomponent oxides. *Catalysis Today* 35(3):247–268.

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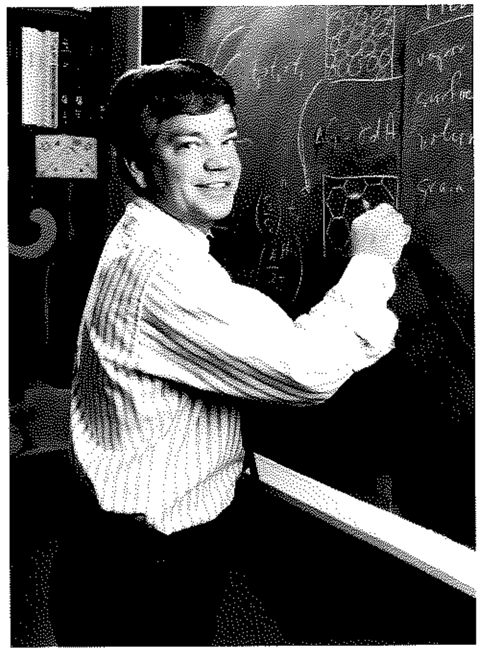
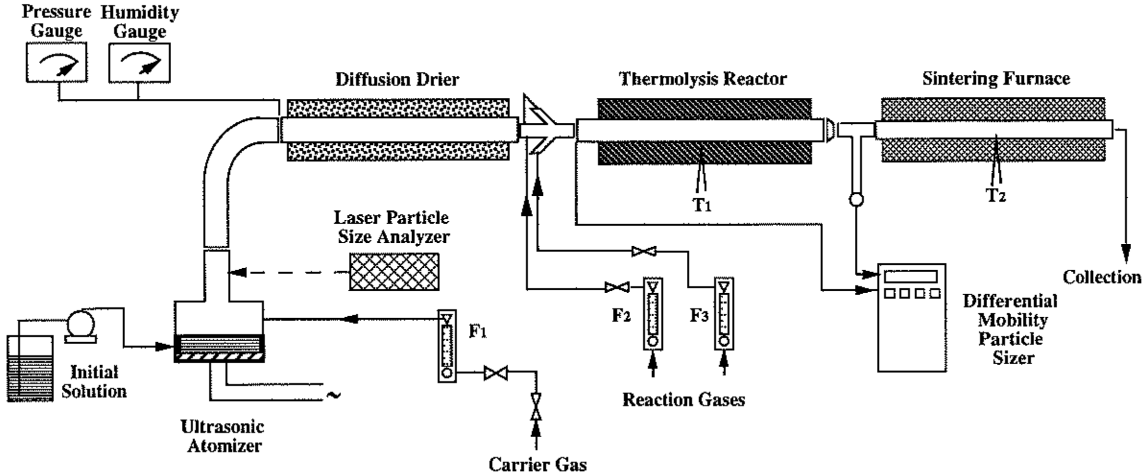


Figure 1. Schematic of spray pyrolysis system.



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Keywords

ceramic processing, powder synthesis, spray pyrolysis, solid-phase epitaxy and phase transformations, sol gels, sintering

Suzanne E. Mohney *Metallization and Oxidation of Electronic Materials*

Professor Mohney is interested in metallization and oxidation for electronic devices. Previously, she has studied thin-film electrical contacts to indium phosphide, which is an important semiconductor for optoelectronic and high-speed electronic devices. The thin-film metal contacts are an essential part of these devices, and controlled metallurgical reactions between the contact and semiconductor are often required to engineer the electrical properties of the contacts. On the other hand, uncontrolled reactions can result in nonuniform or irreproducible contacts and poor thermal stability during processing, packaging, or extended operation of the device. Through an examination of the thermodynamics and kinetics governing the reaction at the interface between the contact and semiconductor, contacts with greatly improved thermal stability, uniformity, and electrical performance can be designed. For the study of electrical contacts to InP, phase equilibria for the relevant metal–In–P systems were calculated or experimentally determined to help understand the reactions between the metals and InP and to suggest thermally stable contact materials. This work also involved the metallurgical and electrical characterization of the contacts, with techniques such as transmission electron microscopy, Auger depth profiling, and glancing angle X-ray diffraction providing detailed information about the metallurgical reaction between the film and semiconductor.

More recently, she has applied these approaches for studying electrical contacts to the wide band gap semiconductors gallium nitride and silicon carbide, which are of particular interest for optoelectronics in the blue and UV wavelengths and for high-temperature electronics. Her research group has also begun to investigate the oxidation of these semiconductors. Additional interests include the study of metal/metal contacts for electrical connectors, particularly in extending the wear of the metal coatings on these connectors.

Publications

B. P. Luther, S. E. Mohney, T. N. Jackson, M. Asif Khan, Q. Chen, and J. W. Yang. 1997. Investigation of the mechanism for ohmic contact formation in Al and Ti/Al contacts to n-type GaN. *Appl. Phys. Lett.* 70:57–59.

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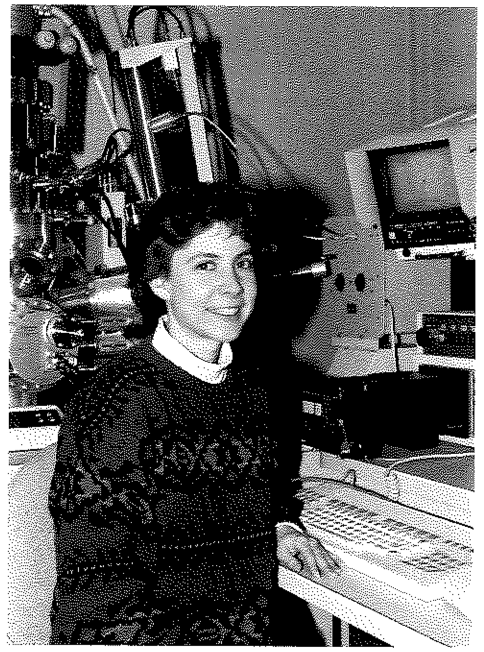

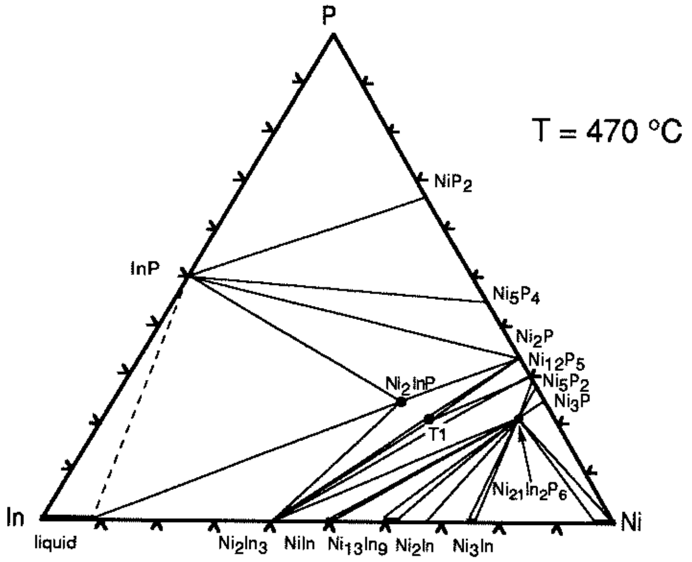

Figure 1. The experimentally determined Ni–In–P isothermal phase diagram aids in understanding the reaction between Ni contacts and the InP substrate. The diagram also shows the phases in equilibrium with the semiconductor InP. These phases may be evaluated for their potential as thermally stable (unreactive) electrical contacts to InP.

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Keywords

thermodynamics, kinetics, interfaces, electronic materials, high-temperature materials, metallization, oxidation

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Robert E. Newnham *"Smart" and "Very Smart" Ceramics*

Robert E. Newnham is Alcoa 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 500 research papers on electroceramics and composite materials for electronic applications. During the past years, he has been awarded the Centennial Prize by the Ceramic Society of Japan, the John Jeppson Medal of the American Ceramic Society, the Turnbull Prize of the Materials Research Society, and the First International Ceramics Prize of the Academy of Ceramics for "distinguished and creative contributions to the advancement of ceramic science and culture, especially in the field of composite electroceramics." Newnham is active in several professional societies, having served as editor of the *Journal of the American Ceramic Society,* President of the American Crystallographic Association, 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 response. It is both a sensor and an actuator. Applications include vibration damping systems for space structures, and energy-saving windows 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 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 property coefficients. 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 forces to control response.

Newnham is currently developing a family of tunable transducers, which utilize the nonlinear properties of relaxor ferroelectrics interleaved with thin layers of rubber and metal end caps. The basic design is patterned after metal–ceramic 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 fre-

Q, the electromechanical coupling coefficient k, the acoustic impedance Z_A, and the electrical impedance Z_E. In the tunable transducer, the magnitudes of f, Z_A, and Q are controlled by stressing thin layers of rubber, while k and Z_E are manipulated by applying bias fields to tape-cast layers of relaxor ferroelectric such as magnesium niobate (PMN). As shown in Figure 2, electrostrictive PMN 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 nanoscale structure and diffuse phase transformations. Under these circumstances the structure is poised on the verge of an instability, and responds readily to external influences such as electric or magnetic fields, or mechanical stress.

Publications

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Figure 1. Flextensional actuators made from poled lead zirconate titante (PZT) ceramics and shaped metal end caps.

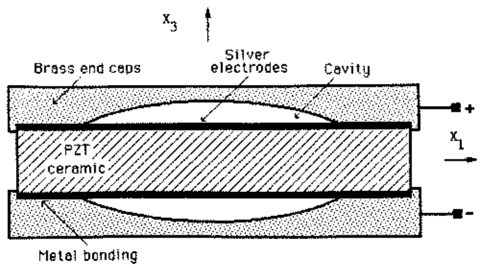
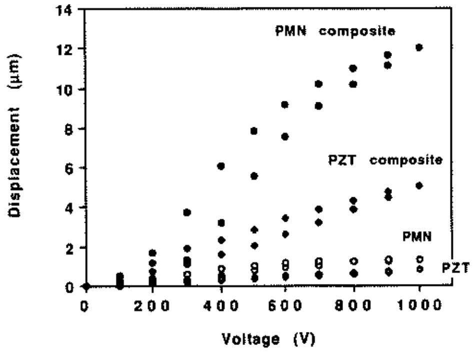


Figure 2. Capped composite actuators made with electrostrictive PMN and piezoelectric PZT amplify the strains of the uncapped ceramics. All four actuators are 1 mm thick.



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Keywords

smart ceramics, very smart ceramics, transducers, composite actuators, sensors

Kwadwo Osseo-Asare

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

Research on particle design seeks to create environments that systematically constrain particle nucleation, growth, and aggregation. In the gel–sol method, highly condensed metal 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. Also under investigation is microemulsion-mediated synthesis where surfactant-stabilized nanosize cavities 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 (electro)chemical behavior of metallic, semiconductor, and insulator materials. Of particular interest are the thermodynamic modeling of the relevant solid–solution equilibria and the elucidation of the roles of metal–ligand complexes, surface complexation, and semiconductor electrochemistry.

Interfacial phenomena underlie many of the techniques available for ion and particle separations. Surfactant aggregation phenomena are under investigation in connection with reversed micellar catalysis of hydrometallurgical liquid–liquid extraction. Polymer–salt interactions can induce phase separations in aqueous systems. Particulate separations that use such aqueous biphases as liquid–liquid transfer media are being developed.

Publications

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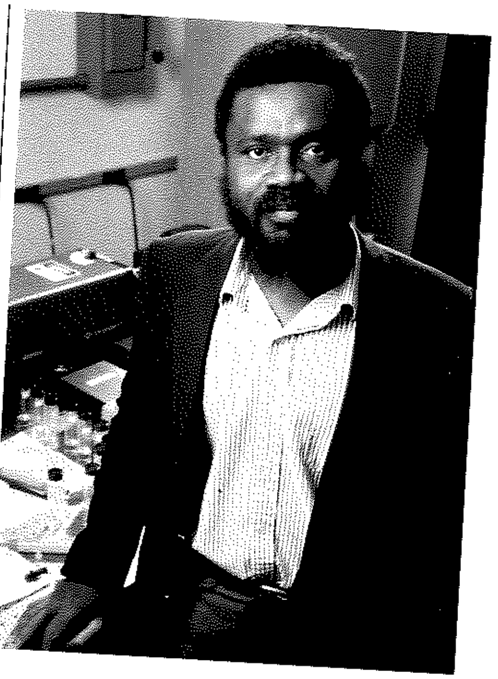

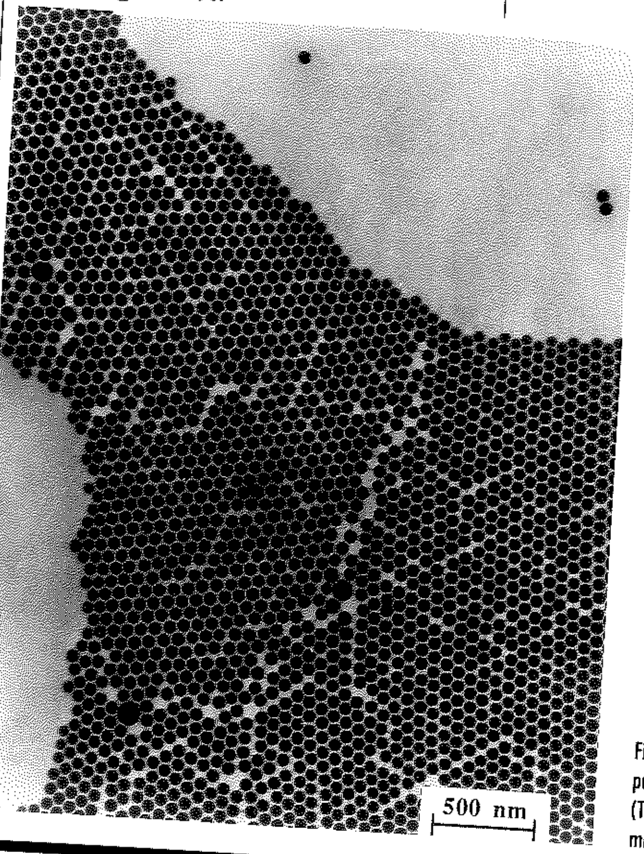

Figure 1. TEM micrograph of SiO_2 particles prepared by hydrolysis of tetraethoxysilane (TEOS) in the NP-5/cyclohexane/NH_4OH microemulsion.

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Keywords

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

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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 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 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 be treated by using the assumption of a chemical equilibrium between the monomolecules 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, 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.

Publications

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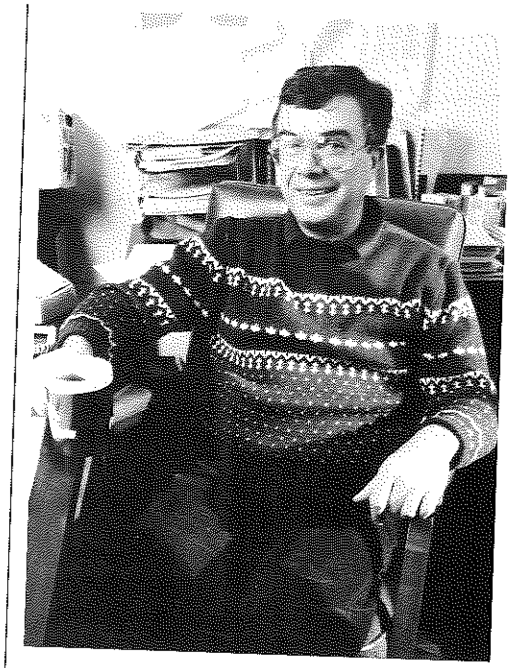

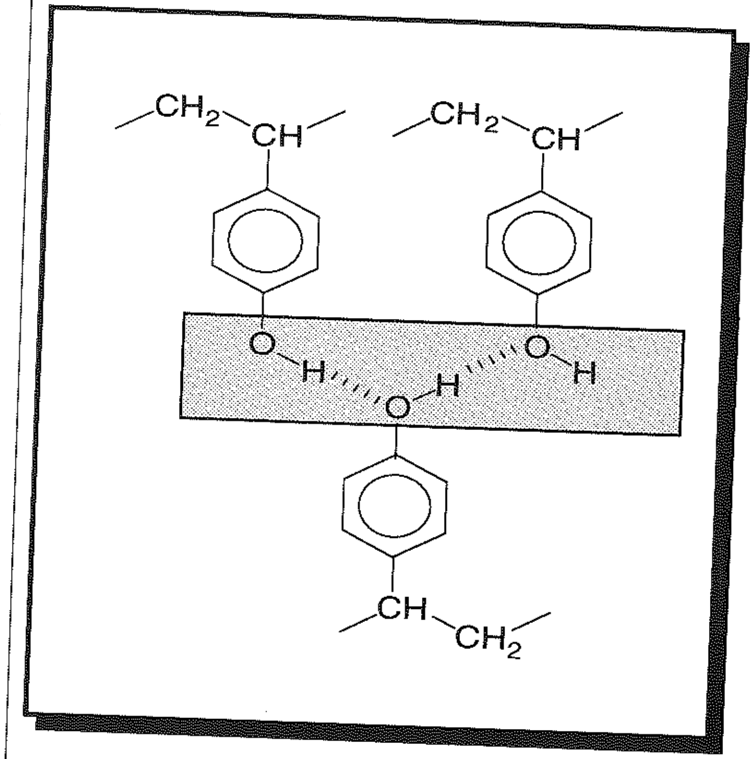

Figure 1. Hydrogen bonding in poly [vinyl phenol].

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Keywords

hydrogen bonding in macromolecular systems (synthetic polymers and coal), polymer blends, gels, liquid crystal/polymer mixtures, coal structure

Carlo G. Pantano

Glass Surfaces, Interfaces, and Thin Films

The surface composition and structure of glass nfluence its adsorption reactions, adhesion, ptical response, and mechanical strength. Needless to say, these chemical properties of lass surfaces and interfaces—which are the ommon denominator in all of Professor 'antano's research programs—exert a profound nfluence upon technological issues including ynthesis of thin glass films for microelectronic pplication, glass/polymer interfaces, glass-maix composites, and the chemical/mechanical urability of commercial glass products.

Whereas the fundamental understanding of omic structure and chemical behavior of etal and semiconductor surfaces is quite rigorus, a comparable understanding has not been hieved for glass surfaces. This situation is obably intrinsic to the nonequilibrium, amorous nature of the glassy state itself. In the se of metals and semiconductors, the scienic understanding has come from a detailed mparison between the surface structure and e bulk structure. By contrast, the bulk structre of glass does not always provide a meangful or convenient reference state. The very ncept of a quantifiable glass structure is still der debate. The approaches to its charactertion to date are neither precise nor definitive, d the kinetics of the glass transition yield a ltitude of metastable states. Thus, it is rdly surprising that most understanding of ss surfaces is empirical.

The empirical approach to control and taiing of glass surface properties has been atly enhanced through the use of surfacesitive measurement techniques. Due to the t that glass surfaces are most often created at vated temperatures, the surface of the glass is lom an abrupt termination of the bulk comition and structure. Thus, the ability to racterize, directly, the surface of glasses is essary in research as well as in process develnent. Pantano and his group are experienced he application of these tools (including S, SIMS, FTIR, ISS, and TPD) to glass—uding commercial glass products. Studies e shown that compositional surface modifion due to the temperature and atmosphere ing processing may extend thousands of stroms below the surface. Moreover, expo- of the surface to humid atmospheres leads progressive in-depth hydration of the glass ace that alters the optical reflectivity, ngth, and adsorptivity of the surface. Conent with these studies of real glass surfaces, ore fundamental definition of glass surfaces been derived through the study of model ces including clean fracture surfaces and oporous sol/gel films. These model surfaces nore suited to the understanding of adsorp- and transport in glass surfaces, and the nanisms through which glass-surface reac- influence the creation of real surfaces

Publications

A. D'Souza and C. G. Pantano. 1997. Determination of the surface silanol concentration of amorphous silica surfaces using static-SIMS. *J. Vac. Sci. Tech.*, in press.

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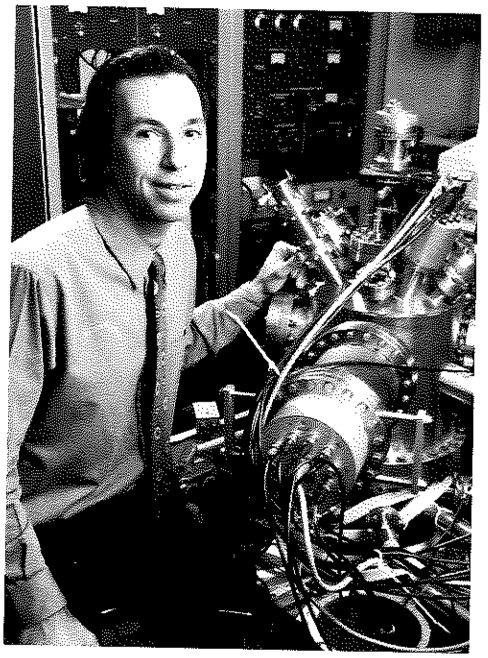

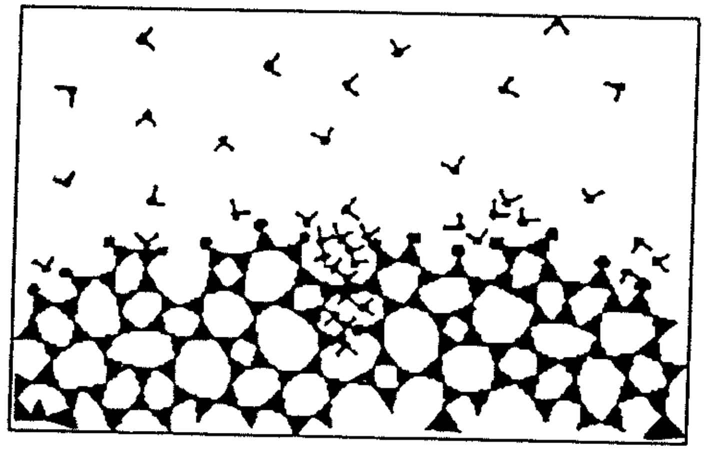

Figure 1. Model of a silica glass surface (in cross section) showing chemisorption, physisorption, and stress-corrosion cracking in a water vapor atmosphere.

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Keywords

glass, surface chemistry, surface analysis, glass/polymer interfaces, sol/gel glasses, glass composites, glass thin films

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Development of Clean Coal Technology

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, clean coal 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 of coal is the formation of nitrous oxide (N_2O). Unlike NOx and SOx, nitrous 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 Pels are centered around developing clean coal technology that incorporates NOx, SOx, and N_2O abatement strategies. His focus is on radiation initiated NOx and SOx emission control and catalytic gasification of coal.

Radiation-initiated removal of NOx and SOx from flue gases is an emerging technology, with a high potential of becoming a competitive alternative to the more traditional NOx and SOx reduction techniques. One of its strongest points is that both pollutants can be efficiently eliminated in a single unit operation. The principle of this technology is that a flue 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 electrostatic field in which a non-thermal plasma is generated. In both cases, fast electrons initiate a series of radical reactions that result in the oxidation of NOx and SOx to nitric and sulfuric acid. By the addition of ammonia, salts are formed that deposit or can be removed from the gas using electrostatic precipitators or bag house filters just as fly ash is removed. The challenge is to manipulate the reaction conditions in such a way that nitrous oxide emissions are also diminished without sacrificing the reductions in NOx and SOx emissions already accomplished.

Coal gasification is one step of the combined cycle technology 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 gases 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 and

Publications

J. R. Pels, F. Kapteijn, J. A. Moulijn, Q. Zhu, and K. M Thomas. 1995. Evolution of nitrogen functionalities in carbonaceous materials during pyrolysis. *Carbon* 33(11):1641–1653.

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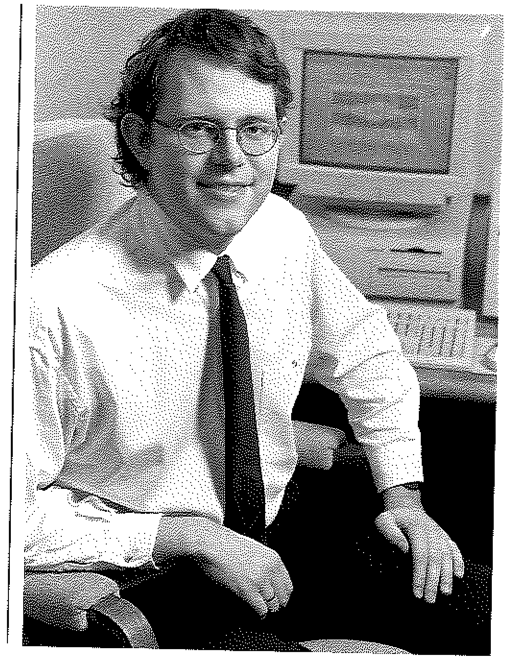

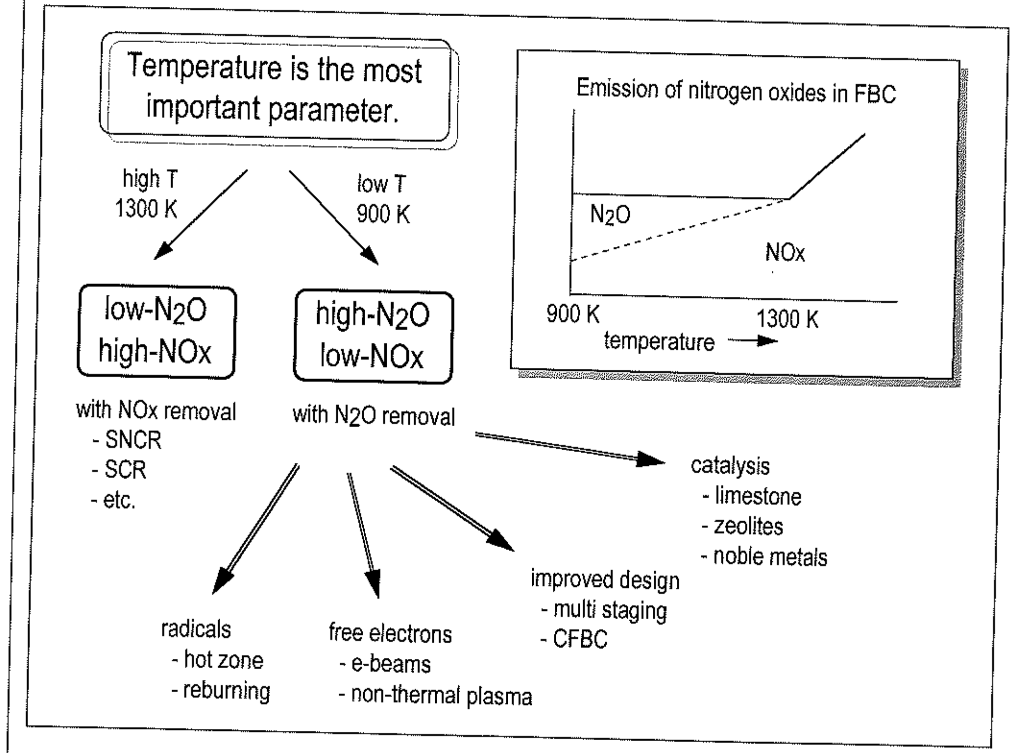

Figure 1. Basic strategies for combined abatement of NOx and N_2O in fluidized bed combustion of coal. By careful selection of a combustion temperature only one nitrogen oxide, either NOx or N_2O, may need to be removed from the flue gases instead of both. Sulfur capture must be included in all cases.

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Keywords

clean coal technology, NOx/SOx abatement strategies, nitrous oxide emissions, catalysis, e-beam, non-thermal plasma, fluidized-bed combustion, coal gasification

oward W. Pickering

Corrosion and Electrodeposition of Metals

ofessor Pickering's teaching and research ac-
ities focus on the principles of electrode reac-
ons and their application (1) to the corrosion
metals and methods for its prevention, and
) to the electrodeposition of metals. The rel-
ant electrochemical (oxidation and reduction)
actions, and the changes that the metal sur-
e undergoes during the reaction, are an im-
rtant aspect. More specifically, research in
r corrosion laboratories includes the study of
) selective element dissolution from alloys; (2)
alized electrochemical-degradation processes
ch as crevice, pitting, and grain boundary
rrosion; (3) reduction reactions including
drogen evolution and its absorption and dif-
sion into metals; (4) development of im-
oved inhibitors for preventing the corrosion
metals and alloys, such as is achieved for cop-
r and its alloys by adding iodide ion to
nzotriozole and other triozoles; and (5) sur-
e reconstruction in metal electrodissolution
d electrodeposition in aqueous solutions us-
scanning tunneling microscopy (STM) and
mic force microscopy (AFM).

lications

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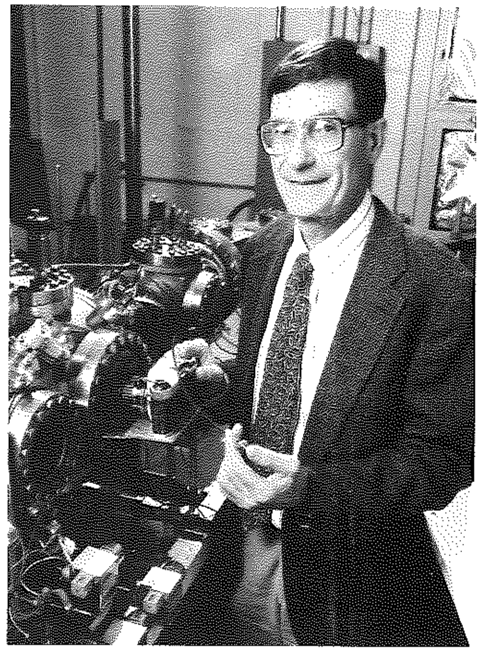

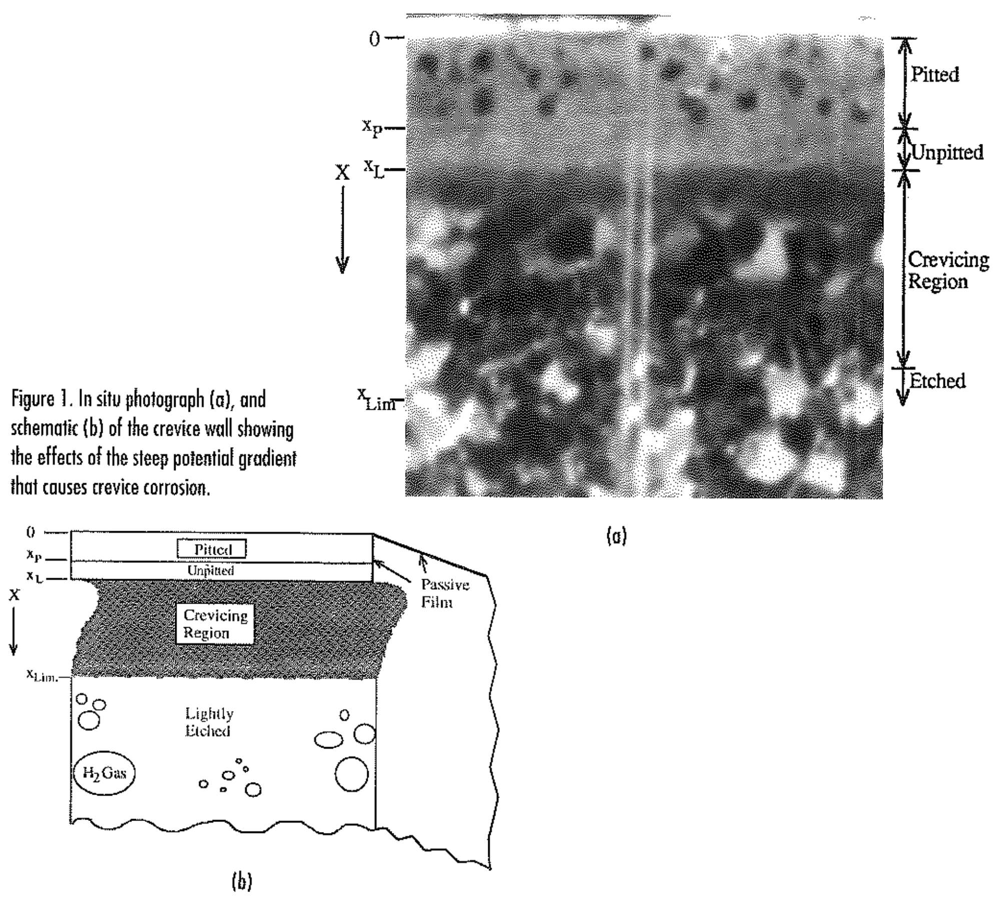

Figure 1. In situ photograph (a), and schematic (b) of the crevice wall showing the effects of the steep potential gradient that causes crevice corrosion.

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Keywords

surface properties, electrode reactions, corrosion of metals, electrodissolution, electrodeposition, scanning probe microscopy

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Sarma V. Pisupati

Emissions Control from Stationary Combustion Systems

Dr. Pisupati's research interests are primarily in studying the effects of fuel properties on combustion behavior in fixed, fluidized, and pulverized modes of combustion, and capturing pollutants from the products of combustion. Specific research topics include: coal-water slurry combustion; combustion behavior of coal blends; sulfur dioxide capture in circulating fluidized-bed combustion boilers using calcium-based sorbents; simultaneous SO_2 and NO_x reduction using biomass-based products; and volatile organic emissions from stationary combustion sources.

Emissions from circulating fluidized bed combustors (CFBCs) are minimized by using calcium-based sorbents to capture the SO_2 produced during the combustion of a sulfur-containing fuel. Properties that are reported to influence sorbent performance are particle size, grain size and texture, pore size distribution, and surface area. The particle size specifications of sorbents for operating CFBCs are design specific. Of particular interest are the fine particles that are smaller than the cut point of the recycle cyclone. The residence time of such fines is equivalent to that of a single pass through the combustor, which limits the contact time for SO_2 capture and often leads to the premature removal of unreacted sorbent from the system. Pisupati and co-workers have recently completed a study on the importance of calcium carbonate content and particle size dependency to the performance of various limestones and dolostones in capturing SO_2 in fluidized bed combustors. Data were obtained in a bench-scale fluidized bed reactor, a pilot-scale down-fired combustor, and a 30 MW(e) CFBC. For larger particles, the slow rate of SO_2 diffusion through the product layer limited the extent of sulfation. Hot-stage scanning electron microscopy and microprobe analysis of the sulfur distribution in the particles indicated that some sorbents developed thermally induced fractures (TIFs), while others with comparable $CaCO_3$ contents did not. The TIFs promoted SO_2 diffusion into the particle and, as a consequence, the sulfation behavior of such sorbents was less particle-size dependent than for those sorbents that did not develop TIFs.

Biomass-based products are being explored for either co-firing with coal or as liquid feedstock for combustion. Biomass-based materials such as BioLime™—an emulsion of calcium and pyrolysis of biomass oil—have shown very promising results as an alternative technology for simultaneous NO_x and SO_2 reduction. This product is introduced downstream from the burner. Ninety percent SO_2 and 50 percent NO_x reductions were obtained simultaneously when firing high-sulfur content coal without combustion modifications for NO_x control. Finely dispersed calcium reacted with SO_2 efficiently, and hydrocarbon radicals from the

rolysis oil reduced NO_x to N_2. It was also observed that overall CO emissions were 20 to 30 percent lower than for coal firing without the injection of this product.

Attempts to reduce NO_x emissions from fossil fuel combustion sources have demonstrated a reduction in combustion efficiency and an increase in the CO and unburnt hydrocarbon emissions. In a current research program, Dr. Pisupati is studying the influence of low NO_x burners on the volatile organic emissions (VOCs) from coal combustion systems.

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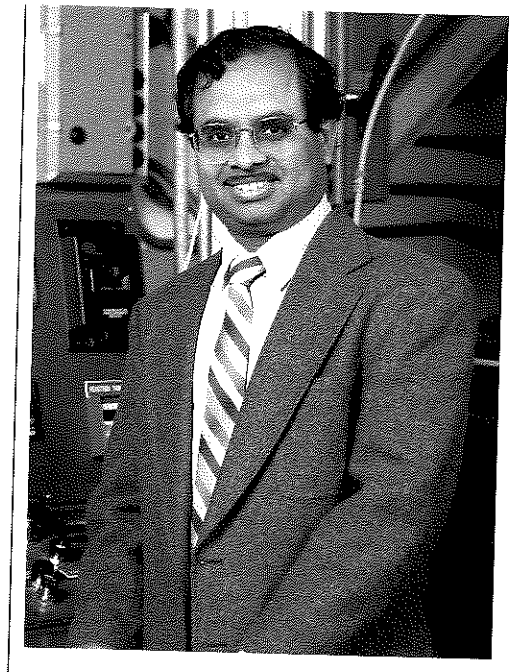

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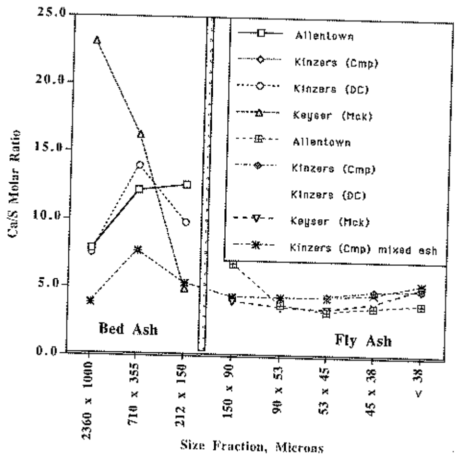

Figure 1. Ca/S molar ratios of bed and fly ashes for various size fractions of selected sorbents in the 30 MW(e) CFBC.

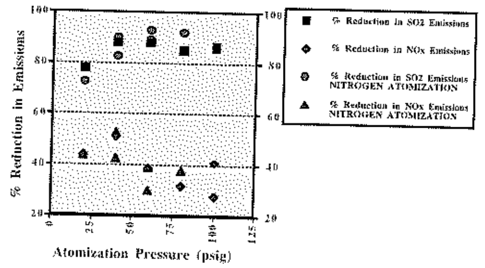

Figure 2. Effect of BioLime atomization medium and its pressure on simultaneous SO_2 and NO_x reduction.

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fluidized bed combustion, SO_2 capture, sorbents, simultaneous SO_2 and NO_x reduction, biofuels

jubisa R. Radovic **Surface Chemistry of Carbon Materials**

ıe performance of carbon materials in many plications depends on their surface proper- s. Here are some examples:

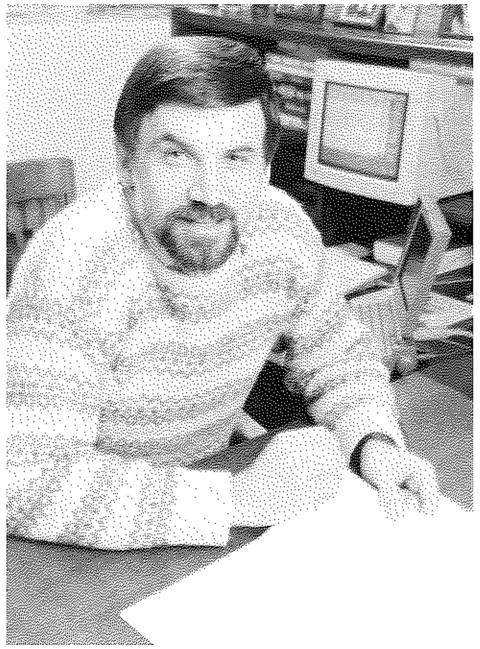
Control of the carbon surface chemistry is ıportant for maximizing the oxidation protec- ın of carbon/carbon composite materials so ese materials can be used as ablative and uctural components in rockets and space hicles. The same chemistry also controls the rameters that lead to the opposite extreme: aximum oxidation reactivity of carbon fuels.

High-surface-area carbon materials are often ımatched in their flexibility as supports for ecious metal catalysts. A suitable pore size stribution of the support is a necessary condi- ın for adequate catalyst performance. The ht surface chemistry is a sufficient condition optimum catalyst performance.

The isoelectric point (pH_{IEP}) of carbon is a y parameter here. Below pH_{IEP}, maximum talyst dispersion and maximum catalytic ac- ity is achieved by using an anionic catalyst ecursor and thus maximizing its interaction th the positively charged adsorbent surface. ınversely, above pH_{IEP}, this interaction is aximized by using a cationic catalyst precur- r.

What does it mean to have the right surface emistry? Figure 1 contains the answer to this estion as applied to the increasingly impor- ıt use of carbon materials as adsorbents in the rification of water. It shows that the frac- ınal uptake of an aromatic pollutant (aniline) n change dramatically as the chemistry of the rbon surface changes. Uptake reduction at v pH is due to electrostatic repulsion be- een the positively charged adsorbent surface d the anilinium cations. Conversion of an nphoteric' carbon (C2) to an 'acidic' carbon 1-E), by surface oxidation, is beneficial be- ıse it decreases this adsorbent–adsorbate re- lsion; but the oxidative treatment of the rface also reduces its π-electron density and ıs decreases the dispersive adsorbent–adsor- te interactions. If the decrease is twofold (C1- D/2), the important net result is enhanced sorption at low pH. But if it is five- or ten- d (C1-E-D/5, C1-E-D/10), the net result at gh pH is suppressed adsorption relative to the se cases (C2 and C1-E).

The simultaneous use of many characteriza- ın techniques is necessary to unravel the im- rtant details of the physical and chemical rface properties of carbon materials. The ones at have been found to provide the lowest st-benefit ratio are: temperature-programmed sorption, electrophoresis, volumetric adsorp- ın, and potentiometric titration.



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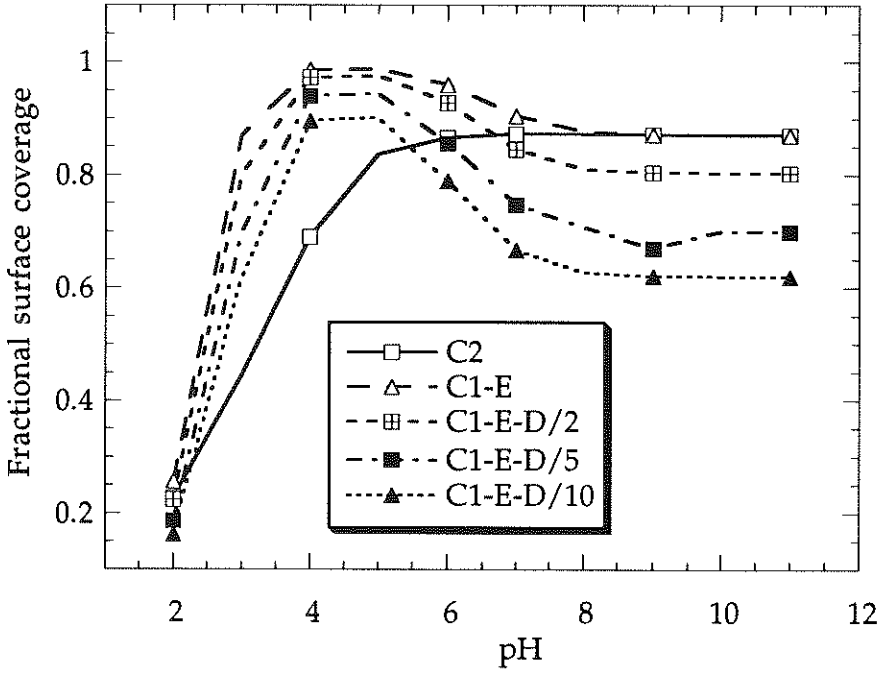

Figure 1. Fractional surface coverage vs. pH for adsorption of aniline from aqueous solution on chemically modified activated carbons.

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Keywords

heterogeneous catalysts, adsorbents, use of carbon materials in air and water pollution prevention, kinetics and catalysis of coal conversion and carbon gasification, methodology of teaching energy supply/demand issues to nontechnical students/general public

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Clive A. Randall **Processing, Microstructural-Property Relations, Theoretical Implications of Microstructural Features in Advanced Electroceramic Materials**

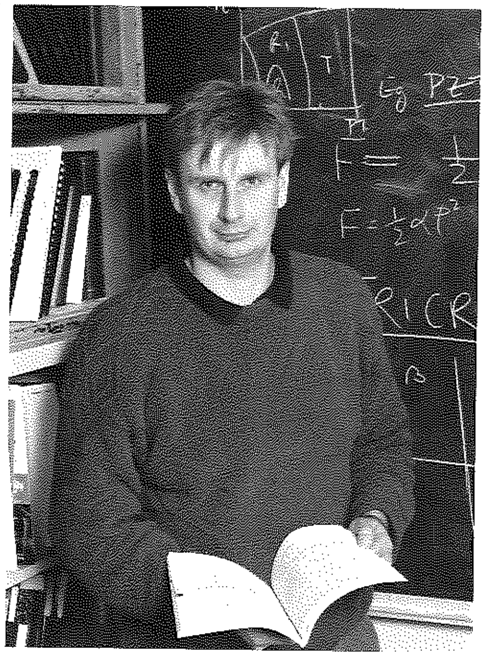
Professor Randall's research interests are in processing and microstructure-property relations in advanced electroceramic materials. Special attention is given to the problems incurred in the optimization and tailoring of elastodielectric properties so as to address issues such as device miniaturization and component integration for higher volumetric efficiencies.

With recent advances in the fabrication of ceramic particulate materials, there exists a need to improve processing assembly techniques to create novel architectures at finer scales. We are investigating the use of electric fields to assemble particulates in composite and thick film form. In general, when an electric field is applied to a stable particle suspension, the particle motion is predominantly dictated by dielectrophoretic and electrophoretic 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 studied in thermoset polymers that undergo in-situ polymerization to produce unique 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 particles into films onto any shaped substrate. By understanding the colloidal stability, the deposition kinetics, and the constrained sintering issues, we have fabricated 1–10 micron $BaTiO_3$ thick-films with high dielectric constant and low losses competitive with other thick-film technologies. The ongoing work is focused on establishing the scientific and engineering aspects of the deposition process. Electrophoretic deposition of electroceramic particulate materials gives potential advances in a number of applications, including piezoelectric motors, biomedical ultrasound probes, and heterojunction chemical sensors.

Ferroelectric and related materials are of interest due to their unique elastodielectric properties that are being used in piezoelectric, electrostrictive, pyroelectric, and capacitive applications. Our group has focused attention on the role of mesoscopic structures on physical properties. Recent work using detailed transmission electron microscopy studies (in-situ and ex-situ) has been on the grain size effects on domain switching mechanisms during poling and defect induced spatial modulations within domain structures, each of which shows a strong influence on the extrinsic property contributions to physical properties. With grain sizes below 1 micron, there is a change in the domain structure and reduction in the number of domain variants per grain; correspondingly there is a reduction in the dielectric and piezoelectric properties. By understanding the dopant effects on mesoscopic structures, we are developing strategies to optimize compositions to establish high-performance piezoelectric properties in sub-micron ceramics.

Similarly, in capacitor materials the kinetic control of the liquid phase sintering process permits a core shell microstructure with heterogeneous dopant distributions. These are processed as to form materials with specific temperature coefficients of capacitance. With submicron grains, the kinetics are more difficult to control. New processing and dopant selection methods are being studied in our laboratory to form specific submicron materials for next generation multilayer capacitors.



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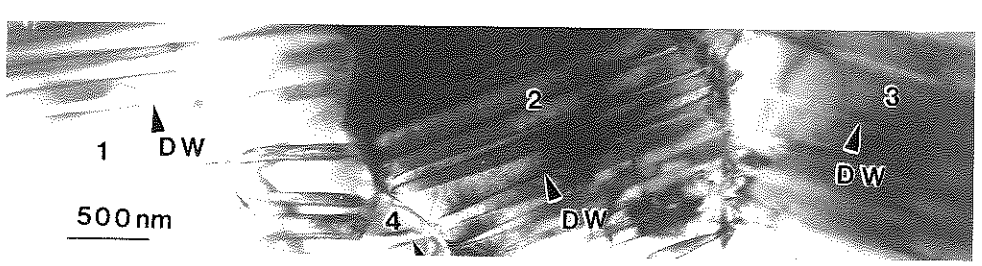

Figure 1. Transmission electron micrograph showing transgranular domain wall coupling in a poled PZT ceramic.

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Keywords

electroceramics, impedance measurements, transmission electron microscopy, composites, thick films

ames P. Runt *Multicomponent Polymer Systems*

mpared to traditional single-component sys-
ıs, mixtures of chemically dissimilar poly-
rs are of considerable technological
portance because of their potential for supe-
r mechanical and physical properties. A par-
ılarly important class of these polymer
nds are those that contain high-performance,
stallizable polymers. In general, Dr. Runt's
earch has focused on developing an under-
ıding of crystallization, microstructure, and
ase behavior in those and other multicompo-
ıt polymer systems, and their relationship to
imate properties.

Some topics of current research interest in-
de: (a) crystalline microstructure (via small-
gle X-ray scattering) and the associated
ıxation behavior of blends of weakly and
ɔngly interacting polymers, (b) the use of
lectric measurements to probe local molecu-
environment and dynamics in copolymers
l polymer blends, and (c) co-crystallization
l phase behavior of homopolymer–copoly-
r mixtures.

In addition, in collaboration with colleagues
he Artificial Organs Section at The Milton
Hershey Medical Center, Runt's research
up has been exploring the properties and
formance of multiblock poly(ether
thaneureas) for use in ventricular assist de-
es and in the Penn State artificial heart. Spe-
cally, the focus has been on (a) the design
characterization of new multiblock copoly-
s with improved barrier properties and (b)
influence of molecular architecture on me-
nical (e.g., fatigue crack propagation resis-
ce) and other properties of poly(ether
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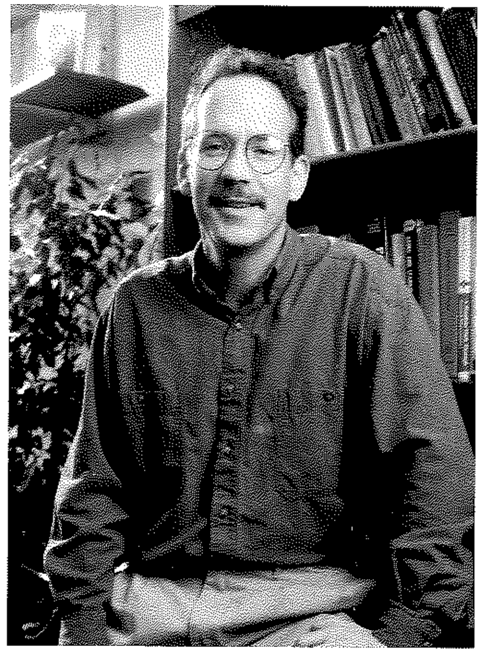

Figure 1. Schematic of three possible microstructures of a miscible binary blend of an amorphous (........) and semi-crystalline (_______) polymer. A. Amorphous polymer is Interlamellar B. Interfibrillar C. Interspherulitic.

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Keywords

crystallization, microstructure, and phase behavior in polymer blends; crystalline polymers; biomedical polymers related to artificial organs (VAD and PSU artificial heart) and orthopedic devices; polymer composites (including PTC materials); electrical and mechanical properties; thermal analysis of polymers; dielectric spec-

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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 stresses gas-phase treatments aimed at the removal of chemical contaminants from the silicon surfaces, and also involves developing tools for gas-phase surface processing in microelectronics manufacturing. In addition, he is actively involved in the development of methods for in-line, 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 (wet) wafer cleaning will remain a dominant cleaning method in this area. However, wet 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 initiated, several years ago. Ruzyllo and his graduate students have participated in this effort since its beginning. They developed the reduced pressure anhydrous HF (AHF)/alcoholic solvent etching of native chemical oxide, as well as the overall dry cleaning procedure involving the following operations carried out in sequence without breaking the vacuum: UV/O_2 + AHF/methanol + UV/Cl_2 + UC/O_2. 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 post-RIE surface processing that includes a UV/O_2 polymer removal process and a UV/Cl_2 "soft etch" of silicon resulting in damage- and contamination-free surfaces.

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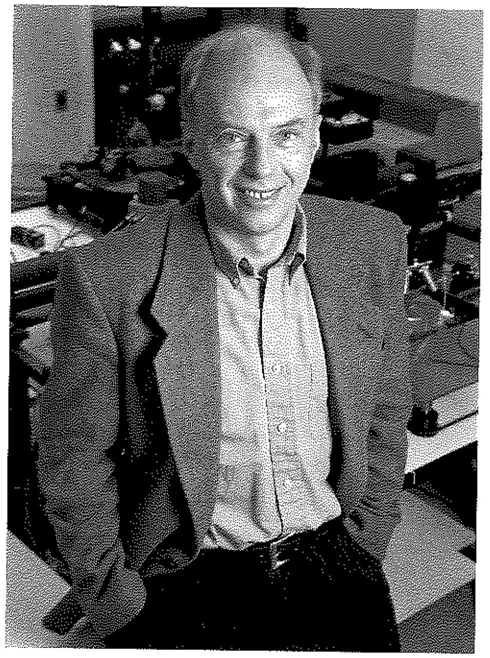

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Keywords

microelectronic processing, silicon, surface cleaning, surface conditioning, in-line process monitoring

Earle R. Ryba *Determination of the Structures of Quasicrystalline Materials*

uasicrystals are materials whose X-ray and
lectron-diffraction patterns exhibit non-crys-
allographic symmetries, such as five-, eight-,
en-, and twelve-fold rotation axes. The five-
nd ten-fold symmetries in the diffraction pat-
erns bely the existence of long-range bond ori-
ntational order in these materials in which the
toms bond along icosahedral and pentagonal
r decagonal directions. While this overall pic-
ure of the connections between the atoms is
nown, the lack of a three-dimensional struc-
ural repeat unit, or unit cell, has made the de-
rmination of the structures of these materials
xtremely difficult. At Penn State, we have been
ctively studying the structure of quasicrystals
nce the existence of these strange materials
as initially announced in 1984.

Recently, our studies have focused on the
ecagonal phase of $Al_{65}Cu_{20}Co_{15}$. Nominally,
e structure of this compound exhibits non-
ystallographic symmetry in two directions,
d a crystallographic repetition along a third
irection. However, from a considerable
nount of X-ray and electron diffraction evi-
ence, we have found that its structure is even
ore complex. Embedded in the quasi-
ystalline structure are extended regions of
sentially periodic atom arrangements, in
hich a very large three-dimensional unit cell
peats dozens to hundreds of times. Further-
ore, these regions of periodicity have been
und to microtwin at angles that are multiples
36°. In addition, the size and shape of the
it cell for the periodically arranged regions
ries, depending upon composition and cool-
g conditions.

We have formulated a comprehensive model
r the structures of this decagonal phase and
e crystalline regions using electron and X-ray
ffraction and the results of high-resolution
ectron microscopy and scanning tunneling
icroscopy studies. This model is built from
ly two primary atomic clusters that are pen-
gonal polyhedra of differing numbers of alu-
inum, copper, and cobalt atoms. These two
usters form aggregates that are easily seen in
e high-resolution electron microscopy and
anning tunneling microscopy images for this
aterial. The possible structural variations,
her periodic or quasiperiodic, based on these
o polyhedra, are numerous. The next ques-
on is how to quantitatively verify the structure
odel.

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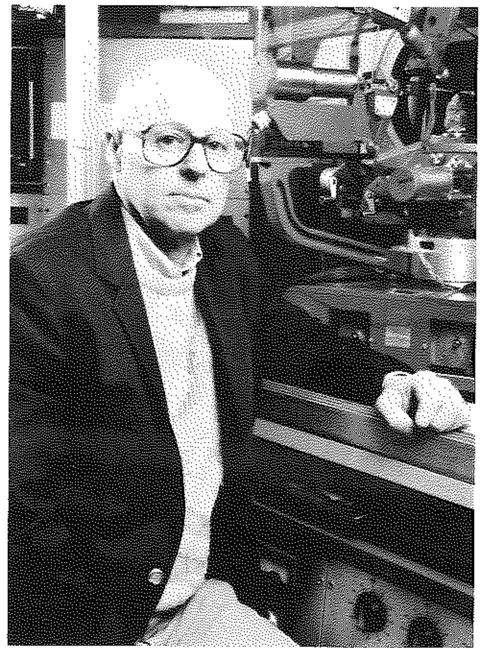

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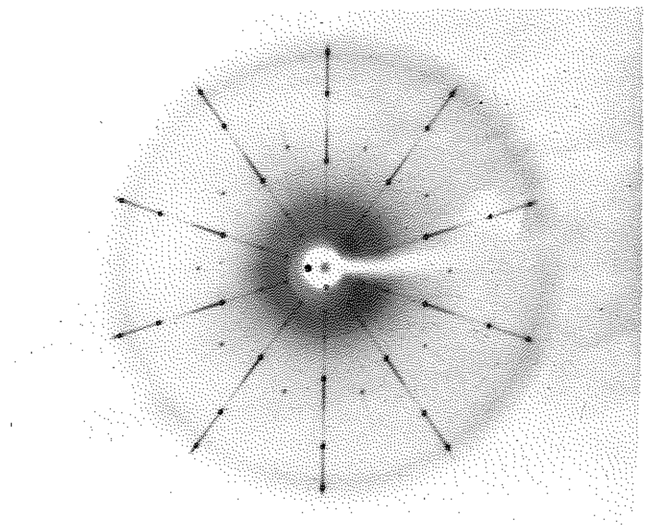

Figure 1. One of the first X-ray diffraction photographs showing non-crystallographic ten-fold symmetry. This X-ray diffraction pattern was obtained from a single fragment of quasicrystalline icosahedral Al_6CuLi_3. Precession photo. MoKα radiation.

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Keywords

X-ray diffraction, structure of thin films and interfaces in composites, grazing incidence diffraction and X-ray reflectivity, structure of intermetallic compounds, mechanism of sintering in powder metallurgy

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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 emission 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 unwanted pollutants and developing technologies for reducing their emission into the environment. A substantial effort has been in the area of sulfur dioxide capture by limestones in fluidized bed combustors. Before the group's research revealed the importance of thermally induced fractures to the efficiency of sulfur capture, limestones were inappropriately specified on the basis of calcium carbonate content. Recent work has shown the importance of grain size in controlling particle attrition, another important aspect of sorbent performance.

Forced oxidation limestone scrubbers are used for post-combustion control of sulfur dioxide in conventional coal-fired power plants. Recent results point to the importance of the dissolution rate of the limestone in the slurry solution 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 ^{15}N NMR spectroscopy to establish the importance of pyrrolic nitrogen in the coal structure as a source of nitrogen oxide. Previous to this pioneering work, pyridinic 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.

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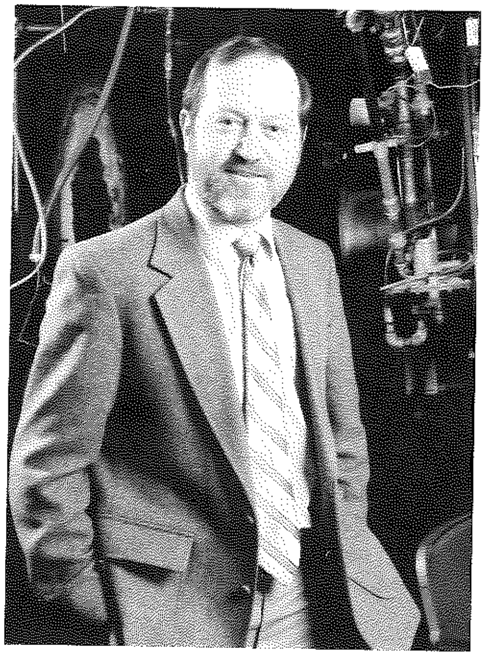

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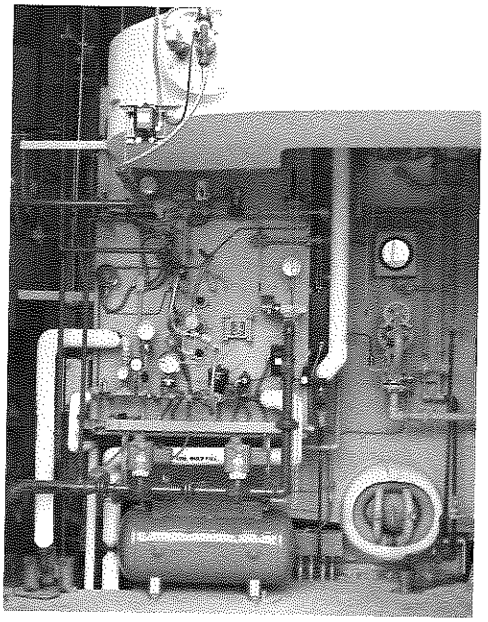

Figure 1. Details of a multifuel demonstration boiler at the East Campus Steam Plant.

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Keywords

coal, combustion, fluidized beds, slurry fuels, combustion-generated pollutants

Darrell G. Schlom *Molecular Beam Epitaxial Growth of Oxide Thin Films*

he focus of my group's research is investigat-
g and perfecting the properties of oxide mate-
als for electronic uses. To do this, we grow
xide thin films on single crystal substrates of
osely related substances. The single crystal
bstrate provides a structural template for the
in films that we grow. The films follow this
omic template and are thus said to be epi-
xial (inheriting their crystalline arrangement
om the underlying substrate). Our focus on
ides is due to the tremendous promise these
aterials hold for electrical applications. Ox-
es exhibit an unparalleled variety of electronic
operties. Insulating, semiconducting, and
en superconducting oxides all exist within the
of structurally compatible oxides known as
rovskites. This structurally related family also
cludes oxides that are magnetic, ferroelectric,
d piezoelectric. In short, this family of oxides
ntains the full spectrum of electronic proper-
s. However, a major challenge is to prepare
ese materials with sufficient quality and inte-
te them with adequate control so that these
operties can be fully utilized in electronic
vices. This is our research goal.

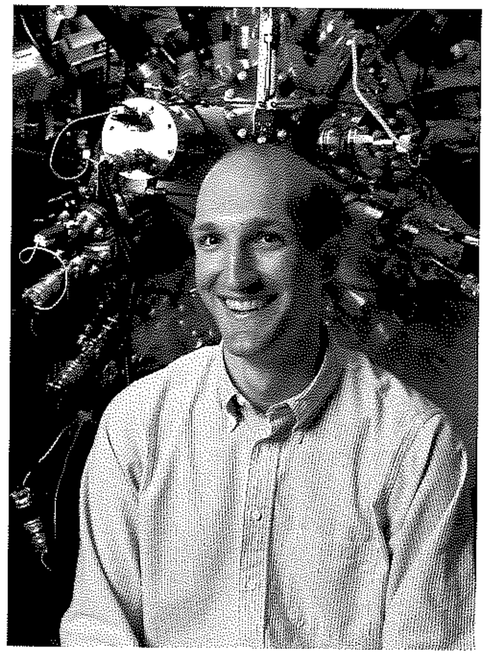
Exploiting the capabilities of these materials
the most demanding electronic applications
l require the synthesis of custom-made stacks
single crystal films, each attached epitaxially
the one beneath it and prepared in such a
y that composition and structure can be con-
lled at the level of single atomic layers. To
ieve this customized layering capability, we
ize a thin-film growth method known as
lecular beam epitaxy (MBE).

MBE amounts to atomic spray painting,
l allows us to prepare customized thin-film
uctures of oxide materials in a very controlled
nner. In this process, several beams, each of
ifferent atomic or molecular type, travel
ough a vacuum of such emptiness (ultrahigh
uum) that collisions on the way to the sub-
te are exceedingly rare, and chemical reac-
ns occur exclusively on the substrate. This
ws beams of highly reactive or even meta-
le species to reach the deposition surface
disturbed. A wide range of growth condi-
ns are accessible using MBE, and such flex-
ity is often key to achieving controlled
wth at the atomic layer level. Several mo-
lar beams may be sprayed onto the surface
e coated, either simultaneously or sequen-
y. The crystalline arrangement of the film
ace is studied during MBE growth with
tron diffraction and after growth by various
acterization methods that allow us to see
tly what the composition of the film is, and
t its properties are (e.g., is it insulating,
iconducting, superconducting, or does it
r performance advantages to existing mate-
and devices?). The nanometer-scale layer-
control allows the growth of customized
ctures in which the sequence of atomic lay-

spectrum of the oxides' electronic properties to be combined in novel epitaxial heterostructures. We recently pioneered the growth of thin films of the ferroelectric $PbTiO_3$ by MBE. This material is important for a new type of high-speed computer memory that does not lose information when the power is turned off.

A second thin-film growth method we employ is a vacuum deposition method called pulsed laser deposition (PLD), in which we vaporize a target made of selected elements with an ultraviolet laser and condense it on top of a single crystal substrate. Although not as precise a thin-film growth method as MBE, PLD offers a rapid means of preparing custom-made stacks of single crystal films. Using PLD, we have recently become the first group in the world to grow thin films of Sr_2RuO_4, the only known high-temperature superconductor that does not contain copper. This material may provide insight into how it is that high-temperature superconductors function.

Our research has so far concentrated on the growth of layered combinations of oxide superconductors and related phases, and ferroelectric thin films. Adapting and applying MBE's layering capability, and the capabilities of the PLD technique, to the controlled integration of other oxide materials will allow the fabrication of novel electronic devices (for example, high-speed, energy-efficient memory for computers). Understanding how to manipulate atoms with ever-greater control to provide enhanced electronic devices is a major goal of our research.



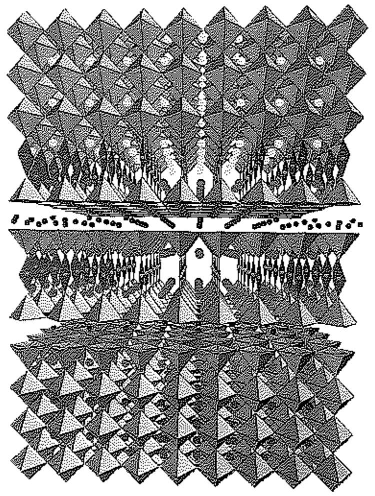


Figure 1. A cross-sectional view of the crystal structure (coordination polyhedra) of a metal-ferroelectric-superconductor field-effect-transistor (MFSFET) heterostructure. The MFSFET consists of a ferroelectric gate insulator ($PbTiO_3$, top), an ultra-thin superconducting channel ($YBa_2Cu_3O_{7-\delta}$ middle), and a substrate ($SrTiO_3$, bottom). The carrier concentration of the oxide superconductor channel layer, and thus its resistance, are modulated by the polarization of the ferroelectric gate insulator. This polarization direction may be flipped by briefly applying a voltage between the gate electrode and the channel. The atomic structure of the interfaces between the oxide layers is a subject of continued study. The interfaces shown are among several proposed possibilities.

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Keywords

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

Harold H. Schobert *Fuel Formulation*

My research interests focus on the chemistry of coal and petroleum (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 aircraft develop significant heat loads from the heat released in the engines. A solution to this problem is to use the aircraft's fuel as a heat sink to cool hydraulic fluids, sensitive electronics, and engine components. The thermal stressing of the fuel in such situations can cause its pyrolytic decomposition, leading to the formation of solid carbon deposits. If these deposits plug fuel lines or burner nozzles in the engine, a catastrophe 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 pyrolytic decomposition regime than current petroleum-only fuels. The key difference is the higher proportion of cycloalkanes and hydroaromatic compounds in the coal-based fuels. Because coals have molecular structures based mainly on polycyclic aromatics, the potential exists to produce highly stable jet fuels by chemically removing the polycyclic aromatic structures from the macromolecular coal structure and hydrogenating them to polycyclic cycloalkanes or hydroaromatics.

Other current research projects focus on the use of coals as feedstocks for the production of graphitic carbon materials; modifying heavy petroleum-derived materials, such as pitches, for production of carbons; and novel approaches to upgrading petroleum residua by direct reaction with methane. Computer modeling of macromolecular structures in coals and neural network computing of viscosities of molten coal ashes are also active projects.

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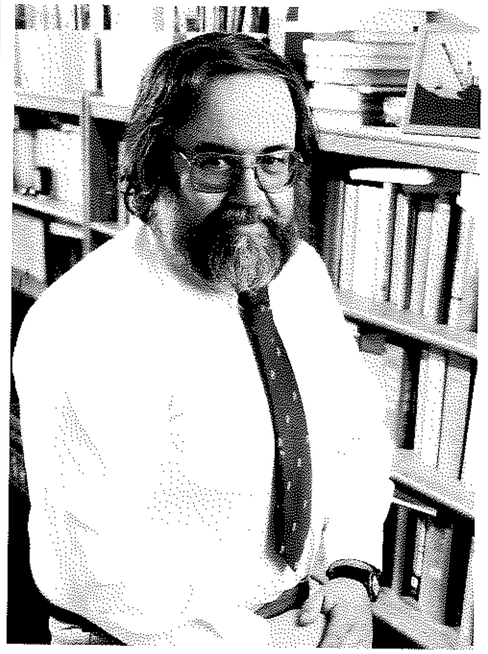
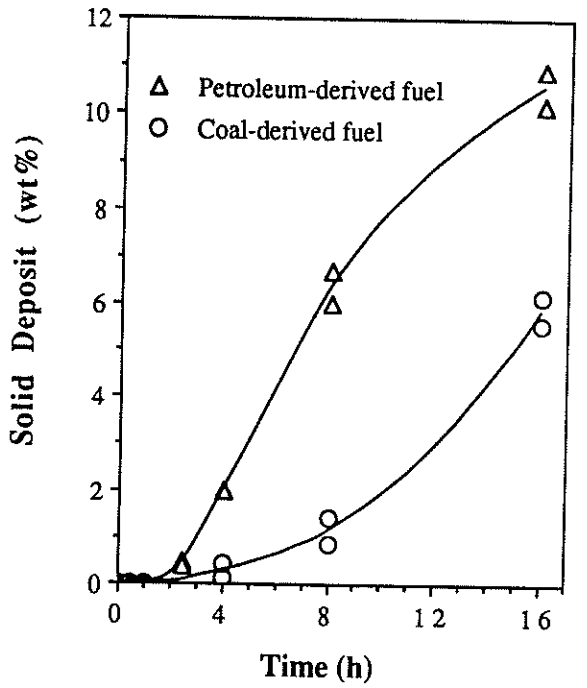


Figure 1. Coal-derived jet fuels are much more stable at extreme temperatures than conventional petroleum-based fuels. This graph compares the breakdown of the two fuels to undesirable solid carbon deposits at 425°C.



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Keywords

jet fuels, coal, coal liquefaction, novel catalysts, coal ash, gasification systems, combustion systems

Chunshan Song *Catalysis in Fuel Processing and Shape-Selective Catalysis*

'rofessor Song's research interests include ıape-selective catalysis for synthesizing spe- ialty organic chemicals, catalysis in fuel pro- essing and energy conversion, synthesis and pplication of novel mesoporous zeolites, and hemistry of high-pressure pyrolysis of hydro- arbons.

Song's research on shape-selective catalysis ocuses on zeolite-catalyzed conversion of olyaromatic hydrocarbons, which has great otential for novel applications. The work on lkylation aims at selectively adding alkyl roups on naphthalene to make 2,6- ialkylnaphthalene, and on biphenyl to make ,4'-dialkylbiphenyl, which are important uilding blocks for advanced polymer materials ıch as high-performance aromatic polyesters nd liquid crystalline polymers. There are many ossible isomeric products from the alkylation, ut only one of them is desirable. The chal- nge is to control the shape selectivity with ertain modified zeolites possessing the desired ore structure and acidic characteristics, with ıe aid of reaction modifier.

In the effort to convert phenanthrene into seful chemicals, Song's group found that some ıordenites and Y zeolites catalyze the ring-shift omerization of sym-octahydrophenanthrene) sym-octahydroanthracene. The latter can be sed for producing anthracene, which is in de- ıand in the chemical industry. Their research n low-temperature hydrogenation of naphtha- ne revealed that mordenite-supported noble ıetal catalysts are much more active and sul- ır-resistant than the corresponding Al_2O_3- or iO_2-supported catalysts. Moreover, shape- lective naphthalene hydrogenation, to either ans-decalin or cis-decalin, can now be hieved. Furthermore, conformational isomer- ation of cis-decalin to trans-decalin was found) occur over certain zeolite catalysts, and mo- cular H_2 dramatically promotes such an omerization.

More recently, Song's group has initiated search on synthesis, characterization, and ıtalytic applications of novel mesoporous zeo- es. This work revealed that certain aluminum ompounds are excellent sources for incorporat- ıg Al atoms into the silicate framework during ydrothermal synthesis, leading to mesoporous uminosilicates with good acidic characteris- cs. There are important catalytic applications ır heavy oil upgrading and fuel processing.

A major challenge in synthetic fuels research to convert coal into liquids at low severity. ecently, Song's group found that using water ıd dispersed MoS_2 catalyst precursor together ould dramatically improve coal conversion ıder H_2 at temperatures that are much lower 25–375°C) than those used in conventional ocesses (400–470°C).

Publications

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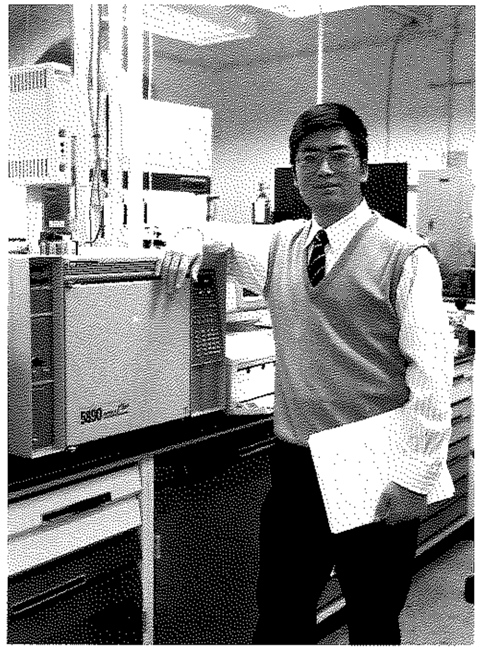

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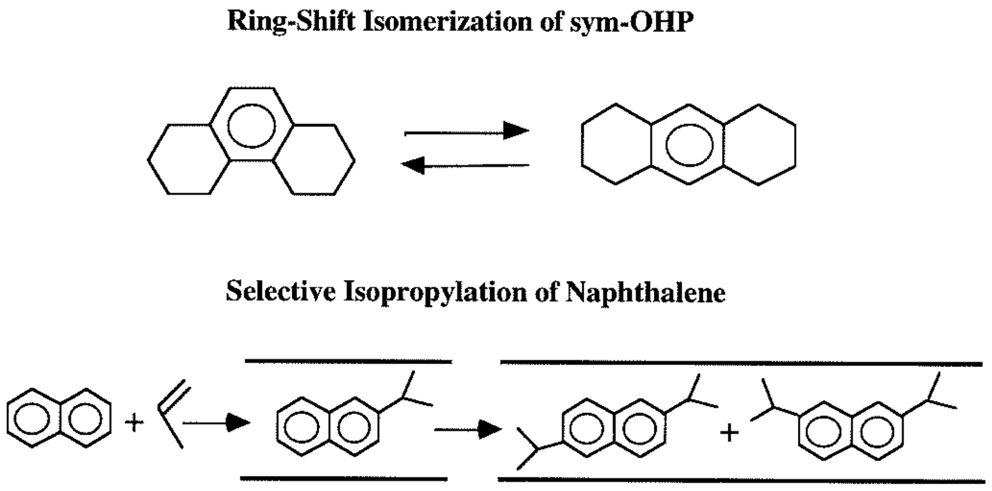

Figure 1. Shape selective isomerization and alkylation reactions over zeolite catalysts.

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Keywords

catalysis, zeolite, alkylation, hydrogenation, isomerization, shape selectivity, fuel, fuel processing, mesoporous molecular sieves, heavy oil upgrading, coal liquefaction, specialty chemicals, high-pressure pyrolysis, jet fuel, thermal stability, reaction chemistry

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Karl E. Spear *High-Temperature Materials Chemistry*

Chemical interactions at high temperatures are critical in the synthesis, fabrication, compatibility, and environmental corrosion of materials. Dr. Spear's research has focused on predicting and understanding the chemical behavior of materials though experimental and theoretical applications of high-temperature chemistry principles, phase equilibria, and thermodynamics. Major areas of research have included nuclear fuel materials, metal boride systems, theory and practice of CVD, oxidation and corrosion, interface reactions in composites, thermochemical analysis of glass systems, and the vapor deposition of diamond.

Spear and his former colleague Michael Frenklach began developing molecular-level models for CVD diamond synthesis in 1985 using atomic models of diamond surfaces, kinetics and mechanisms of hydrocarbon reactions, and steric considerations of gas-surface processes. This research resulted in an experimental process and a patent for homogeneously nucleating and growing submicron diamond powder, the discovery and classification of new polytypes of diamond, and a cyclic CVD process that separates the growth and etching-cycle chemistries. This latter process was modeled to predict the effects of cycle variables on growth rates and deposition quality. Problems with the adhesion of diamond coatings to tungsten carbide cutting tools was approached by first depositing interlayers with compositions based on phase equilibria and thermodynamic modeling.

The utilization of CVD phase diagrams and other thermochemical modeling techniques was developed to predict and explain complex deposition chemistry in boride, carbide, nitride, silicide, germanide, and oxide systems. Such models have proven to be extremely valuable in examining sensitivity and trends in deposition behavior to controllable experimental parameters. Partial equilibrium concepts have allowed the application of equilibrium thermodynamics to these dynamically reacting, nonequilibrium systems. The principles behind the vapor deposition modeling have also been applied to modeling the oxidation of silicon carbide- and silicon nitride-containing systems and composites in research programs directed by Spear with colleagues Dr. Richard Tressler and Dr. Carlo Pantano. Baseline data for understanding the passive oxidation behavior of these materials, and for understanding interface reactions in composites, was developed and modeled. The complex thermochemistry of glass systems is currently under development using the ideas and experiences from previous research on the chemically complex systems described above.

Publications

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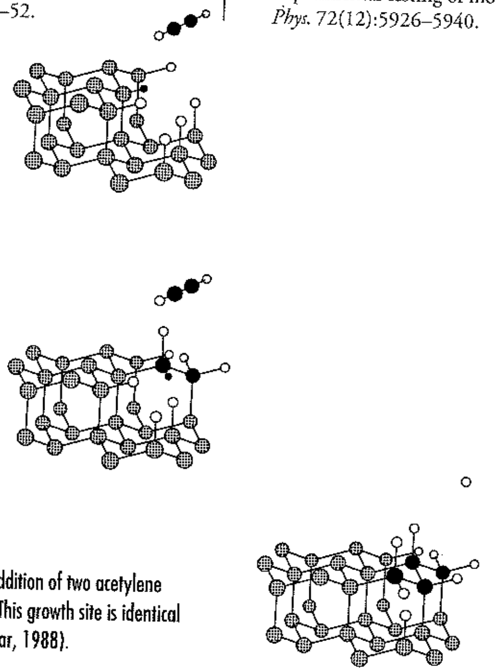

Figure 1. Schematic illustration of the addition of two acetylene molecules to a diamond {110} surface. This growth site is identical to a {111} step site. (Frenklach and Spear, 1988).

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Keywords

high-temperature and solid-state chemistry, thermodynamics and phase equilibria applied to materials synthesis and behavior, experimental and thermochemical modeling of vapor deposition processes, experimental and thermochemical modeling of glass systems, corrosion, chemical reactions at interfaces

eter A. Thrower

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

spite of their excellent high-temperature me-
nical properties, carbon–carbon composites
limited in applications by their oxidation
avior. Inhibiting the oxidation is a major
that may be tackled by either a protective
ting or an inherent modification of the
cture of the material. The incorporation of
on during processing has been explored via
ious routes, and later work has focused on
properties of a new material, BC_3, with the
e crystal structure as graphite. Preliminary
lts indicated that BC_3 has superior oxida-
resistance to graphite (Figure 1), and excel-
t mechanical properties.

Oxidation of carbon–carbon composites
depends on the manufacturing technique
I or pitch impregnation) and the type of
r used. The existence of synergism between
components in the composite is quite clear
ler some circumstances where the reactivity
he composite cannot be determined by add-
the behaviors of fibers and matrix. A sys-
atic study of various fiber–matrix combin-
ns is currently in progress that should help
point the circumstances under which benefi-
synergism exists.

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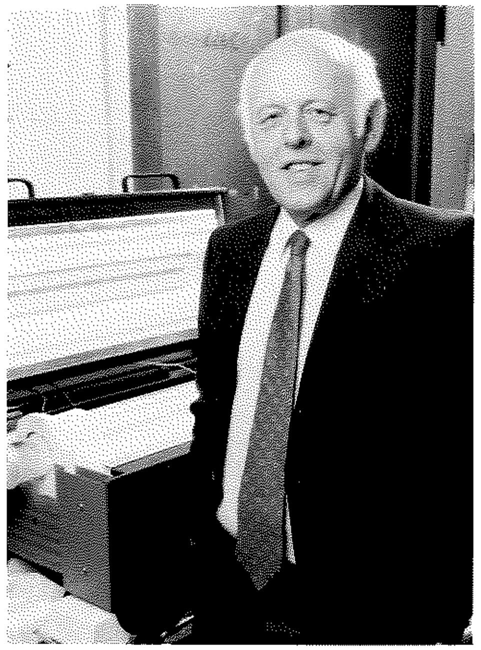

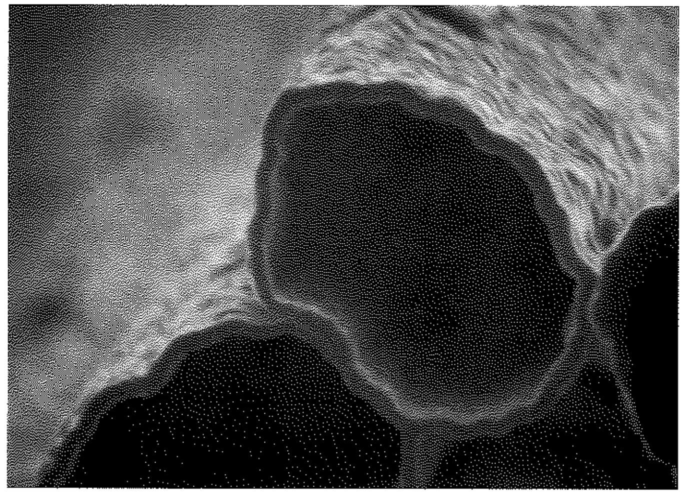

Figure 1. Carbon fiber coated with BC_3 and then oxidized to remove the fiber. The oxidation resistance of the coating is evident.

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Keywords

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

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Richard E. Tressler

Degradation of Ceramics, Fibers, and Composites

In many energy conversion systems and high-temperature processing plants, 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 schemes can best be developed when the processes that control the corrosion and substrate 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–ceramic composites under static or cyclic stresses at elevated temperatures is of major importance for most energy-usage or energy-recovery applications. The fundamental understanding of the failure processes, and the materials characteristics that control these processes, is in the very early stage of development. The design data base of reliable tensile properties of commercially available materials must be developed to assure timely application of these materials.

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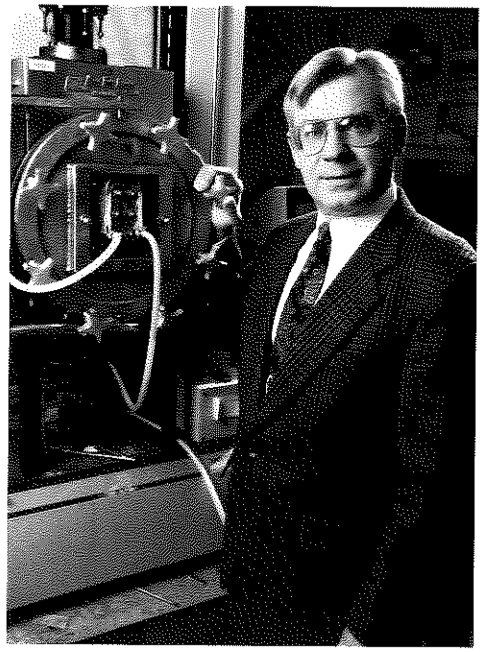
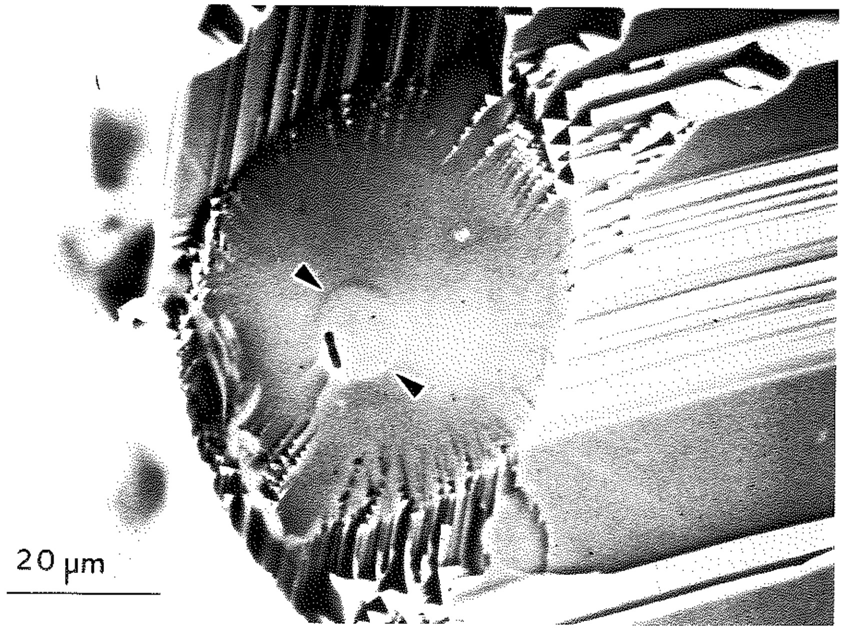


Figure 1. Fracture mirror on the fracture surface of a sapphire fiber tensile tested at 1400°C. There is a region of slow crack growth around the failure origin, a pore.



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Keywords

point defect and impurity diffusion in ceramics; properties of oxide films on silicon-based ceramics; processing of fibers, composites, and in situ reinforced ceramics; oxidation, corrosion, creep rupture, crack growth

Susan Trolier-McKinstry

Structure–Microstructure–Property Relations in Electroceramic Films

Dr. Trolier-McKinstry is interested in the development of electronic ceramics as active materials for sensors and actuators. Her current research program is focused on (1) understanding the factors that control the dielectric and piezoelectric properties of ferroelectric thin films, (2) developing a new family of piezoelectrics based on textured ceramics, and (3) exploiting spectroscopic ellipsometry as a characterization tool for electroceramic films.

Thin film actuators based on $PbZr_{1-x}Ti_xO_3$ or $PbZrO_3$ offer a considerable improvement over the currently used material, ZnO, in terms of both the effective piezoelectric properties and the available energy density. As a result, they would significantly facilitate the development of miniature pumps, microphones, motors, and other active devices. However, due to the combination of extremely small grain sizes, large inherent stresses, and microstructural or compositional inhomogeneities, most thin films do not display the same properties as bulk materials of the same composition. Dr. Trolier-McKinstry's group is working on developing an understanding of the factors that control the properties of ferroelectric films, as well as creating a materials database for designers of microelectromechanical systems. Toward this end, they are using several different types of thin film deposition systems (including sol-gel, pulsed laser deposition, magnetron sputtering, and ion beam sputtering) and are developing new facilities for measurement of fundamental elasto-dielectric properties of thin films (see Figure 1).

One of the primary characterization tools that her group is using as a probe of the microstructure and inhomogeneities present in thin films is spectroscopic ellipsometry. Spectroscopic ellipsometry (SE) is a nondestructive technique capable of depth profiling the dielectric function of materials with an angstrom scale resolution over a depth comparable to the penetration depth of light in the material. In the case of ferroelectrics, this means that SE bridges the gap between existing tools designed to characterize either the bulk or surface of ceramic 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 the superconductor $YBa_2Cu_3O_{7-x}$, the significant oxygen sensitivity of SE is being used to study oxygen diffusion real-time in thin films. This should enable an improved understanding of the critical factors affecting the properties of superconducting junction devices.

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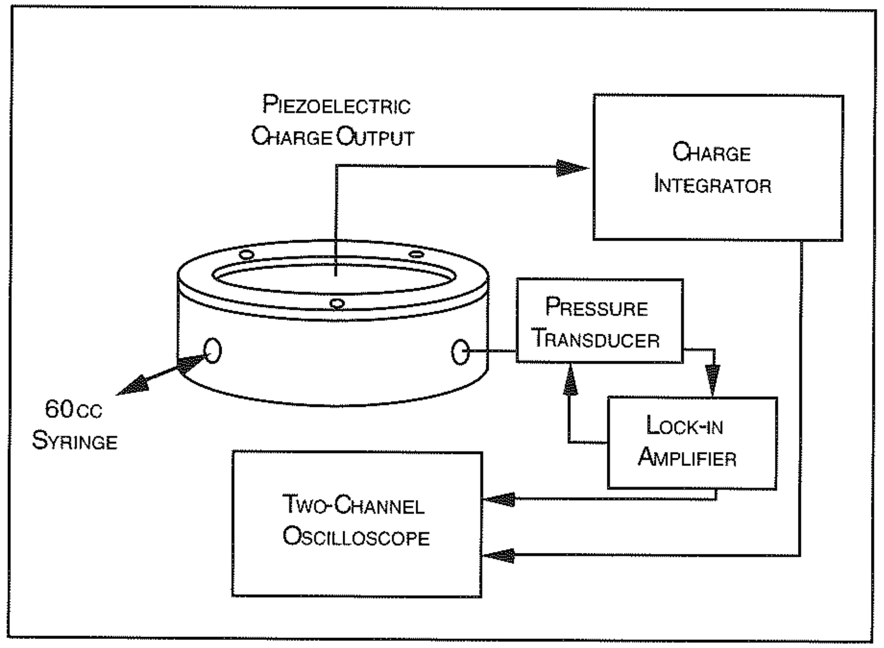
Figure 1. Schematic of a new measurement tool for determining the piezoelectric charge coefficient d_{31} of thin film transducers.



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Keywords
ferroelectricity, spectroscopic ellipsometry, thin films, electroceramics

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Walter A. Yarbrough

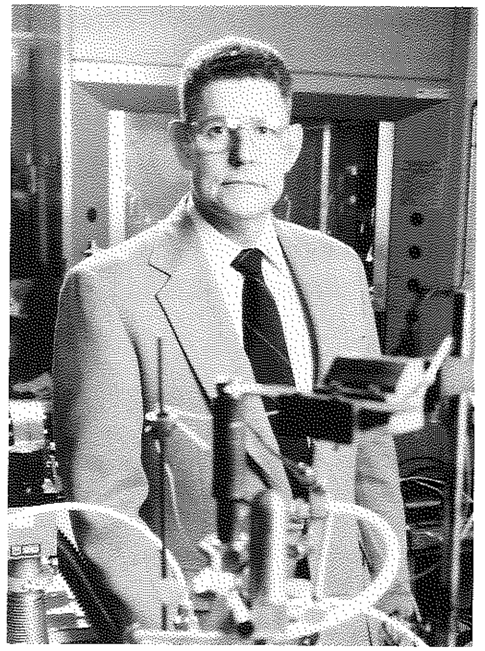
Synthesis and Preparation of Materials

Professor Yarbrough's major research interests are in the synthesis and preparation of materials. A major focus continues to be how microstructural development and phase-formation processes in the fabrication of materials are influenced by the presence of surfaces and interfaces. These interests include the nucleation and growth of both stable and metastable phases. He and his students have recently concentrated on the synthesis of metastable phases, principally diamond and cubic boron nitride, through the use of chemical vapor deposition (CVD). Although early reports from Russia and elsewhere that well-crystallized diamond could be synthesized using CVD met with considerable skepticism, by 1984 it became apparent that these 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 kbar. Thus, Yarbrough and his students are focusing on two major issues.

The first of these issues is the question of why well-crystallized diamond should 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 crystalline perfection of the solid diamond formed in CVD? Closely related to this is the second issue: Can other similarly valuable but metastable crystalline phases be synthesized using CVD and related methods? This issue has practical importance in that the answer would help in selecting potentially fruitful approaches for novel materials' synthesis and fabrication. Paramount among the other materials of interest is the ultrahard, high-band, gap refractory semiconductor cubic boron nitride. Like diamond, cubic boron nitride is extremely valuable technologically and is also a high-pressure phase, metastable at atmospheric pressure. Unlike diamond it is not available naturally and can only be reproducibly prepared at very high pressures.

In the effort to provide answers to these questions, Yarbrough and his students have pursued theoretical and experimental work on the synthesis of metastable phases by CVD. Yarbrough has shown that a well-crystallized metastable phase (e.g., diamond), may indeed be thermodynamically preferred over the conventionally accepted stable phase. This is because, in most processes, crystal growth occurs by the addition of material to the solid surface. If bulk recrystallization or transformation is sufficiently inhibited, then phase control can be established at the solid surface (i.e., the interface between the crystal and the reactants contributing to growth). Thus, the relative stability of the bulk phase may at best be irrelevant, and at worst misleading, to the researchers inter- Yarbrough has shown that the relevant thermodynamics rationalizing the formation of diamond use thermodynamic potentials appropriate for the solid surface in local equilibrium with vapor or liquid 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 concentrations, the diamond surface structure is more stable than that of graphite. For example, the dominantly observed surface of graphite, the (0001) or basal plane surface, is thermodynamically preferred relative to the commonly observed (111) surface on diamond at low atomic hydrogen concentration. However, when the atomic hydrogen concentration is higher than that expected at true thermostatic equilibrium, the diamond surface is indeed preferred to the graphite surface.

The successful use of this formalism as a guide to understanding the growth of diamond implies a useful paradigm in materials synthesis: If reconstruction or transformation in the bulk solid can be ignored, as is true with many refractory phases, control of the solid structure can be achieved by adjusting synthetic parameters to control the surface structure during the crystal 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 cubic structure during nucleation and growth. Research exploring this and other similar possibilities is continuing.



Publications

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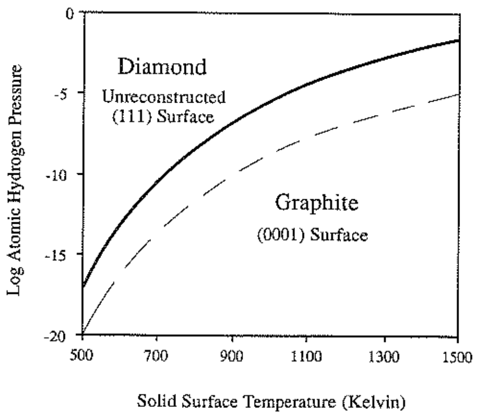

Figure 1. Results of calculations comparing commonly observed surfaces of diamond and graphite. It is generally recognized that the unreconstructed octahedral or (111) surface of a diamond crystal is most often terminated by chemisorbed hydrogen. This surface consists of a "puckered" hexagonal array of carbon atoms, and as such is quite similar to the hexagonal array or "sheet" of carbon atoms that form the (0001) basal plane surface of graphite. At low atomic hydrogen partial pressures for a given temperature, including those expected at global equilibrium (the dashed line), the preferred surface structure is that of graphite. At high atomic hydrogen partial pressures, such as might be expected if a nearby continuous source of atomic hydrogen is present, the expected surface structure switches to that of the diamond surface. The dark continuous line represents the boundary between the conditions where the diamond and graphite surfaces are preferred.

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