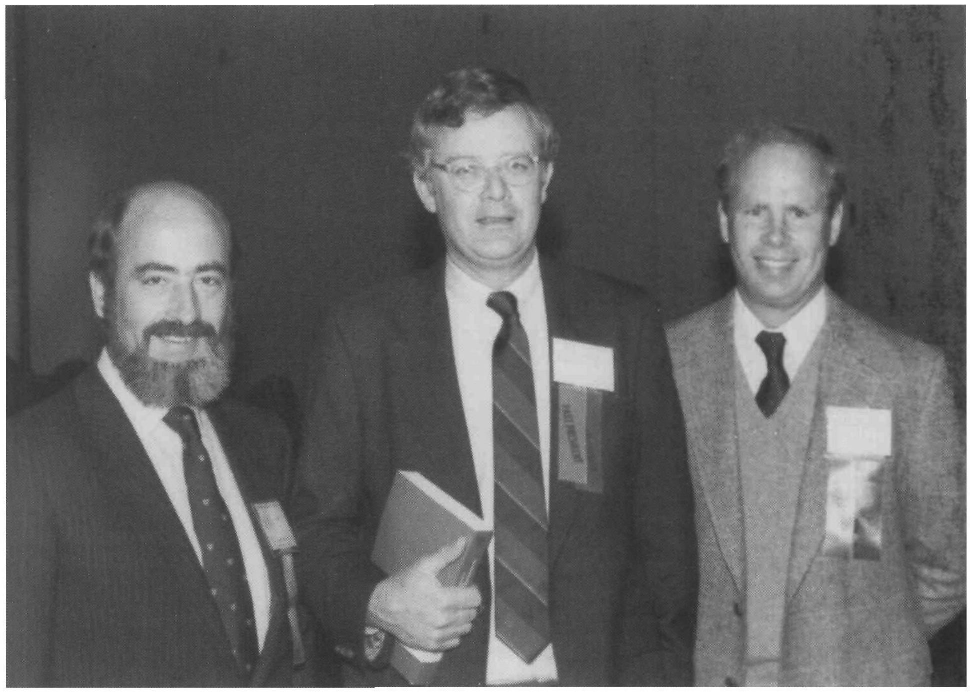
Beam-Solid Interactions and Phase Transformations (Symposium A)

Symposium Organizers: H. Kurz, Technical University Aachen, G.L. Olson, Hughes Research Laboratories, and J.M. Poate, AT&T Bell Laboratories.



Symposium A Organizers (left to right): H. Kurz, J.M. Poate, and G.L. Olson.

This symposium was devoted to the fundamental aspects of beam solid interactions and beam-induced phase transformations in materials. The symposium began with a full-day plenary session organized jointly with the symposium on Beam-Induced Chemical Processes. This session consisted of eight invited papers by internationally recognized scientists who reviewed recent work in the fields of laser-solid and surface interactions, ion-solid interactions, and phase transformations. The final two days of the symposium consisted of both oral and poster sessions on the interaction of photon, ion, and electron beams with solids and the thermodynamics and kinetics of rapid phase transformations between metastable and stable states.

The plenary session was particularly honored to have presentations by two speakers who had given invited papers at the first laser annealing symposium in 1978. N. Bloembergen from Harvard University reviewed the current understanding of the dynamics of laser-induced phase transitions, primarily melting and evaporation, in the microsecond to femtosecond time regimes. D. Turnbull, also of Harvard University, discussed the thermodynamics and kinetics of the transitions between the crystalline, liquid, and amorphous phases of Ge and Si. In the morning session, C. V. Shank (AT&T Bell Laboratories) reviewed recent studies of the dynamics of ultrafast processes which occur during pulsed laser irradiation of solids. He showed that the dynamics of lattice heating in the picosecond range are governed by the Auger recombination process. He also discussed the first measurements of the thermalization of electronic carriers in multiquantum well structures. Helmut Walther (Max Planck Institute) and Y. R. Shen (University of California) reviewed recent progress in studies of molecule-surface interactions and nonlinear optical processes at surfaces. Dr. Walther discussed time-of-flight measurements of NO molecular scattering at surfaces. The dynamics and energetics of the scattering process for incident molecules in the v+0 and v+1 vibrational states were presented. In addition he reviewed recent experimental studies of the structure and orientation of absorbed molecules which were performed using a new laser-driven tunneling microscopy technique. Prof. Shen discussed how nonlinear optical techniques can be used for in-situ measurements of surface structure. Surface second harmonic generation was emphasized, and it was shown how this technique can be used as a surface probe with submonolayer sensitivity.

In the afternoon session, Walter Brown (AT&T Bell Laboratories) presented a review of the fundamental processes operative during ion-solid interactions. He highlighted progress in studies of collision cascades, ionization spikes, and energy transfer which occur when energetic ions interact with solids. J. S. Williams (Royal Melbourne Institute of Technology) described recent work on the kinetics of solid phase crystallization and diffusion in amorphous silicon. The dynamics of solid phase processes which occur during furnace heating were contrasted with the dynamics of ion-induced solid phase transformations in amorphous silicon. J. W. Mayer (Cornell University) concluded the plenary session with a discussion of phase formation and ion beam mixing in alloys. Particular attention was paid to the formation of equilibrium and metastable phases formed by ion beam mixing in multiple layer samples, and the formation of quasicrystalline Al(Mn) alloys by ion irradiation.

The four topical sessions in the symposium were devoted to the areas of laser-induced melting and excitation of semiconductors, laser-induced phase transformations in carbon and metals, ion beam-solid interactions, and ion beam mixing and metastable phase formation. Studies of phase transitions and melting of graphite received considerable attention at this symposium. Work on this new topic was presented by speakers from MIT, Harvard University, AT&T Bell Laboratories, and Bell Communications Research. The investigations were centered around whether the phase transition in graphite results in a metallic liquid or an insulating molten phase. Although important new information was provided at the meeting, this issue is as yet unresolved and remains an active research topic. A second new area which was highlighted in the symposium concerned the kinetics and mechanisms of ion-induced crystallization. R. G. Elliman (CSIRO, Australia) and G. Holmen (Chalmers University, Sweden) presented data which suggest that deposition of energy via nuclear collisions at the crystal/amorphous interface is the dominant process in ion-induced epitaxy. Dr. Elliman showed that in contrast to results obtained for conventional furnace annealing, the rate of ion-induced epitaxial grow this not influenced by either the substrate orientation or the presence of doping impurities in the amorphous film. He suggested that the major fraction of the "thermal-only" activation energy for epitaxial crystallization of Si is associated with formation of nucleation sites at the interface, a step which is achieved athermally by the ion irradiation process. Investigators from MIT and the IBM T. J. Watson Research Center showed in related paper show ion irradiation can be used to enhance grain growth and control the crystallographic orientation of thin films.

A topic which has recently received considerable research attention is the forma-

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tion of a new quasicrystalline phase possessing long-range orientational order but lacking translational symmetry. The production and characterization of this new icosahedral phase was reviewed by J. A. Knapp (Sandia National Laboratories). Both pulsed e-beam heating and ion beam mixing were used to form the quasicrystalline phase in Al(Mn). The effect of temperature during ion beam mixing on the formation of the new phase was described by Dr. Knapp and subsequently by D. A. Lilienfeld (Cornell University). The temperature dependence for the amorphous-to-quasicrystalline transition and the composition range over which the transformation occurs were discussed in terms of a model for energy exchange and defect evolution during ion beam mixing in the Al (Mn) system.

In summary, the symposium addressed important fundamental issues relating to beam-solid interactions. In addition to excellent review papers describing the current status of research relating to photon, ion, and electron beam interactions with solids, new developments in these areas were presented in the more than 60 contributed papers presented at the oral and poster sessions at the meeting. The symposium not only showed how our understanding of many processes has matured over the last eight years, but also indicated how this understanding is leading to exciting new developments in this expanding field.

Symposium Support: Air Force Office of Scientific Research (K. J. Malloy), Army Research Office, Materials Science Division (J. Hurt), Office of Naval Research (L. R. Cooper), and Hughes Research Laboratories.

Proceedings: Volume 51 of the Materials Research Society Symposia Proceedings series.

Rapid Thermal Processing (Symposium B)

Symposium Organizers: T. O. Sedgwick, IBM T. J. Watson Research Center; T. E. Seidel, J. C. Schumacher Company; B-Y. Tsaur, MIT Lincoln Laboratory

Symposium B on Rapid Thermal Processing became at this Meeting a dynamic and growing offspring of the traditional Symposium A. Symposium B brought together research activities ranging over a variety of materials and processes, but all focused on using broad area heat sources to anneal and process materials over relatively large areas (100 cm^2) and for short times (seconds). Interest in rapid thermal processing RTP), which has been hosted from its inception by MRS, has grown dramatically from just a couple of papers in 1981 to 59 invited and contributed papers in Symposium B at this Fall Meeting. Tom Sedgwick, Tom Seidel, and Bor-Yeu Tsaur, all of whom have made leading edge contributions in semiconductor materials and device studies involving RTP, were symposium organizers.

The materials were, of course, the focus at the 2½ day symposium. Silicon and silicon transistor technology dominated with its host of associated materials, vis., oxides, nitrides, silicides, and reflow glass. The session on compound semiconductors was dominated by GaAs and related III-V materials. The rapid annealing process, which started a few years ago as an outgrowth of laser annealing with a focus on ion implant damage removal, has now grown to include "processes" with reactive gases such as oxidation of silicon, the nitridation of oxides, and now the use of RTP to grow epitaxial silicon, which was reported first during this meeting by C. M. Gronet and co-workers from Stanford University. This technique resulted in minimal autodoping and may, in fact, herald the introduction of RTP "style" processing equipment to carry out a wide range of semiconductor processing steps. As the move toward larger wafer sizes continues and if single wafer processing becomes pervasive, it would seem likely that many device fabrication steps will be carried out in equipment of the rapid-thermal-processing type which can minimize thermal cycle and provide rapid process turnaround.

There were many new results reported in Boston; only a few can be mentioned here. A. E. Michel of IBM, in an invited paper on diffusion in silicon, presented data on a long (hours), low-temperature (800°C), transient diffusion in boron-implanted samples that can lead to very deep (hundreds of nanometers) junction motion. This huge diffusive motion is related to a smaller transient diffusion seen in RTP samples which can be dramatically reduced by annealing with RTP rather than a furnace but with carefully chosen parameters. E. Myers and co-workers from North Carolina State University reported on a new "reverse amorphization" phenomena where highly damaged crystalline silicon becomes amorphous at very low temperatures. The first really extensive temperature studies of RTP using two imbedded thermocouples in a wafer show interesting and important transient thermal effects in RTP processing according to R. Sheets of Tamarack Scientific Corporation.

Fundamental studies relating to solid-state processing in short times were also the subject of several presentations. The first extensive data on solid-phase epitaxial growth of amorphized GaAs, a subject important in RTP of ion implanted contacts and junctions in GaAs, was presented by Y. I. Nissim of CNET, Paris. M. L. Reed and J. D. Plummer of Stanford used RTP to measure the kinetics of silicon/silicon dioxide interface trap removal. These and other studies on oxidation kinetics show how rapid thermal processing equipment can be used to extend the range of high-temperature process studies to much shorter times.

The pace of Symposium B was changed on Tuesday evening when a panel of experts in semiconductor processing and RTP equipment manufacturing were brought together (with ample refreshments) to confront the question "Where Will Rapid Thermal Processing Be Required for VLSI Processing?"

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Symposium B Organizers (left to right): T.E. Seidel, T.O. Sedgwick, and B-Y. Tsaur.

Equipment Exhibit.

with Tom Seidel as moderator. The panelists and the audience engaged in wide ranging and sometimes spirited discussion, although the topic question was not directly answered.

As summed up by Tom Sedgwick, the RTP community is still very heavily engaged in working out the details of RTP process control and material studies. It has become clear that in an RTP reactor many materials and processes important to semiconductor fabrication can be carried out. What is not clear is to what extent the use of RTP offers a unique or distinct overall advantage compared to standard processing. P. K. Vasudev of Hughes pointed out that the ideal place to introduce RTP into manufacturing is in a process that is relatively uncritical and insensitive to time and temperature control. His comments are dramatically underlined by the fact that RTP has been introduced for the glass reflow step on the essentially completed device structure by several manufacturers. The pros and cons of using RTP for oxidation and for silicide formation were vigorously debated. The use of RTP for shallow junction formation seems to be waiting for more detailed materials studies but particularly more device results. Other factors such as single wafer processing and rapid turnaround processing may also become important in determining when RTP will become important in manufacturing.

Symposium Support: A. G. Associates, Eaton Corporation, Tamarack Scientific Corporation, Varian Corporation; Army Research Office, and Office of Naval Research.

Proceedings: Volume 52 of Materials Research Society Symposia Proceedings series.

Beam-Induced Chemical Processes (Symposium D)

Symposium Organizers: R. J. Von Gutfeld, IBM T. J. Watson Research Center; J. E. Greene, University of Illinois; H. Schlossberg, Air Force Office of Scientific Research.

The symposium on Beam-Induced Chemical Processes, organized by R. J. Von Gutfeld, J. E. Greene, and H. Schlossberg, was comprised of six invited and 58 contributed papers during a 2½ day forum. The primary issues addressed ranged from photo-stimulated surface processes, deposition, and etching to the role of ion/surface interactions during vapor phase crystal growth.

As was evident from the number of papers presented and the ensuing discussion, there is a rapidly growing interest in the development of photo-initiated dry processes for custom metallization in integrated circuits, making and breaking links in multi-level metallization, and mask repair. Several papers were concerned with the problems involved in direct writing as well as projection patterning of metal lines from spin-on organometallic polymers. The lowest resistivities were generally obtained at the lowest scan rates due to incomplete reactions at high scan velocities. Increasing the laser power or operating at too long a dwell time resulted in non-uniform film thickness due to desorption and evaporation from the center ("hot spot") of the irradiated region.

The use of spin-on inks such as dimethyl gold acetate which decompose through strongly exothermic reactions can also result in the uncontrolled generation of large periodic features as a result of reaction front running ahead of the laser beam. Better results were obtained with Pd-acetate in which Gross from AT&T reported minimum line widths of 1.8μm and a resistivity of $\geq$5 times that of pure bulk Pd for writing rates of ~100m/s. In all cases, however, the films still contained significant concentrations of silicon, oxygen, and carbon. Chapman et al. (Lincoln Laboratories) described a scheme for restructurable VLSI based upon the application of laser linking to wafer-scale integration.

Several papers discussed the deposition of metal films by laser-assisted chemical vapor deposition (LCVD) from metal-alkyl, carbonyl, and metal-halide donor molecules. Most of the experiments were carried out using pyrolysis although in some cases, such as W deposited from $W(CO)_6$ using an Ar^+ ion laser operated at 350-360 nm (Gilgen et al., Columbia University), the process was initiated photochemically. Film resistivities within a factor of two of bulk W were reported in the latter case. More fundamental studies were carried out by Bartosch et al. (Cornell University), who used a combination of TSD, AES, and HREELS to investigate the decomposition of $Fe(CO)_5$ chemisorbed on Si(100)2x1 surfaces following irradiation by 257 nm photons from a frequency doubled Ar^+ ion laser. The Colorado State University group of Yu et al. presented data for the growth of a variety of transition metals, oxides, and nitrides by photolytic and pyrolytic CVD.

Some interesting results on the growth of high-quality semiconductor films by LCVD and the use of excimer laser pulses for substrate cleaning prior to epitaxial growth were also presented. Branz et al. from MIT demonstrated and controlled growth of P and B doped a-Si:H films. The partial pressure of the dopant gases was found to affect both the deposition rate and the incorporated H concentration. Undoped films were found to be more intrinsic than glow-discharge deposited a-Si:H. Irvine et al. (RSRE) reported the photo-assisted MO-CVD growth of epitaxial $Hg_{1-x}Cd_xTe$ at temperatures less than that obtainable by normal MO-CVD. $Hg_{1-x}Cd_xTe$ films were grown on CdTe/GaAs substrates with 77 K mobilities up to $5.5 \times 10^4 cm^2/V$-s.

Laser-induced photolytic, pyrolytic, and photo-electrochemical (PEC) etching of metals (Al and Cu), semiconductors (Si and IIIV), and dielectrics (SiO_2 and Si_3N_4) was also reported. Lum et al. from AT&T demonstrated the PEC production of holographic gratings in InGaAsP/InP distributed feedback lasers. Gratings were obtained with a period of 0.35 μm and a depth of

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1000 Å by the interference of two laser beams at the surface of a sample immersed in an electrolyte. The interference pattern produced a sinusoidal variation in the etch rate R where R was proportional to the hole concentration at the solid/electrolyte interface. Experimental data were fit using a two-dimensional hole transport model. Takai et al. from Osaka University obtained 0.7 μm line widths in GaAs and InP by pyrolytic etching in Cl-containing atmospheres using Ar^+ ion laser.

Selective dry etching of III-V alloys using photogenerated carriers to promote surface reactions was discussed by Ashby from Sandia National Laboratories. Photolytic etching of SiO_2 by IR multiphoton dissociation of F containing gasses was reported by Barnnon and Chang of IBM. Johnson et al. of Sandia described a novel bilayer resist which involved the use of an excimer laser for bond scission and patterning of alkyl-substituted polysilanes.

A number of researchers, such as Osgood et al. from Columbia University, investigated various combinations of photo-induced and plasma etching. Okano et al. from Toshiba demonstrated anisotropic photochemical etching of Si using Cl and/or F-containing radicals generated in a microwave discharge, and a one megabit DRAM cell pattern was produced. Fundamental studies of the role of ion/surface interactions during dry etching were reported by McNevin of AT&T who used modulated-beam mass spectrometry to investigate the etching of InP in a Cl_2 atmosphere during bombardment by rare gas ions.

Finally, Sundgren and Greene (Linköping and Illinois Universities, respectively) discussed recent results in the investigation of low energy (~20-500 eV) ion/surface interactions during crystal growth from the vapor phase. Data were presented demonstrating large effects in all stages of film growth including nucleation kinetics, growth kinetics, and elemental incorporation probabilities. In the latter area, changes in ρ by up to 10 orders of magnitude were reported for accelerated ionized dopants in both Si and GaAs. The use of accelerated dopants was also found to result in much sharper doping profiles. Data were fit using a model which included both thermodynamic and kinetic components and accounted for the role of surface segregation.

Principal Symposium Support: Air Force Office of Scientific Research.

Supplemental Support: IBM Corporation

Extended Abstracts: Published by MRS as Vol. EA-5.

Symposium D Organizers (left to right): J.E. Greene and R.J. von Gutfeld.

Thin Films— Interfaces and Phenomena (Symposium E)

Symposium Organizers: R. J. Nemanich, Xerox Palo Alto Research Center; P. S. Ho, IBM T. J. Watson Research Center; S. S. Lau, University of California at San Diego

The symposium was organized to address the properties of thin films with respect to interfaces and related phenomena. The major emphasis was on films interacting with semiconducting substrates. Thin films on both silicon and compound semiconductors were presented. The scientific issues ranged from basic properties of materials to materials issues of specific device structures. The symposium included 16 invited presentations, 66 contributed oral papers, and 53 contributed poster presentations. A notable high point of the symposium was the combined session on Wednesday with the symposium on Layered Structures and Epitaxy (Symposium H).

As in past Thin Films and Interfaces symposia, a large fraction of the work was on silicide formation. The initial reaction at transition metal-silicon interfaces and a theoretical description of the electronic states were described in invited presentations by G. W. Rubloff and O. Bisi. The formation of silicides by interfacial reactions was the subject of several contributed papers. While the reaction kinetics of a wide range of metal overlayers was reported, significant emphasis was noted for nickel, palladium, and titanium films and their reaction products. The reactions can also affect the substrate properties, and an invited presentation by I. Ohdomari described the dopant redistribution as a consequence of the reactions. The formation of silicides by ion-beam mixing was the subject of some controversy; there was apparently a 25-cent wager placed by S. S. Lau. The ramifications of the wager were described in an invited talk by J. W. Mayer.

The interface reactions and kinetics of a wide range of other materials were also presented. The properties of metastable phases were described in an invited talk by F. W. Saris. The effects of interfaces on oxidation and growth of a variety of materials were presented. The growth studies were complemented by a wide range of analysis techniques which included atom probe and ellipsometry in addition to more common interface probes. Of course, electron microscopy was pervasive throughout the symposium.

Of particular interest throughout the symposium were the formation and properties of epitaxial layers. Significant advances in the properties of epitaxial insulators were reported. Invited presentations by L. J. Schowalter and T. P. Smith addressed the UHV growth of CaF_2 lattice matched to silicon to form complicated multilayered structures, and the electrical characteristics of the CaF_2/Si interface.

A wide variety of epitaxial silicides were summarized by L. J. Chen, and several contributed papers also addressed the subject. The combined session with the Layered Structures and Epitaxy Symposium addressed the issues of Schottky barrier formation and epitaxial silicides. The electrical characterization of the interface states

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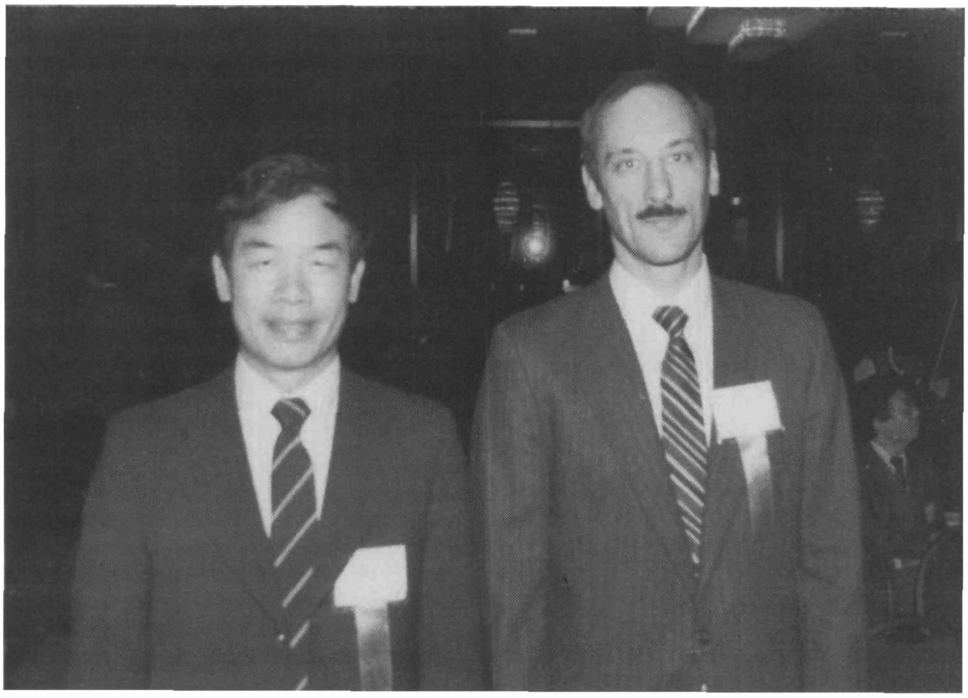

Symposium E Organizers (left to right): P.S. Ho and R.J. Nemanich.

and the silicide film properties were described in invited presentations by E. S. Yang and J. C. Hensel. A contributed paper by C. B. Duke (Xerox Webster Research Center) provided theoretical insight into Schottky barrier formation. A controversial aspect of the Schottky barrier of epitaxial films was the focus of invited talks by R. T. Tung and P. S. Ho. These presentations outlined research progress in understanding the unusual Schottky properties of the $NiSi_2/Si<111>$ interface. Several contributed papers addressed aspects related to key issues of the problem. The major issue is centered on whether the Schottky barrier is intrinsically dependent on the atomic microstructure or the degree of perfection at the interface.

With GaAs devices becoming a reality, the properties of contacts to compound semiconductors is of increasing importance. The interdiffusion and microstructure of the contacts were described in invited talks by L. J. Brillson and T. S. Kuan. The reactions at compound semiconductor interfaces were found to be more complicated than those for group IV semiconductors, but experimental efforts using state-of-the-art surface analysis techniques are bringing new understanding to the problems. Invited presentations by S. Furukawa and N. Yokoyama addressed issues of ion-beam mixing techniques and refractory silicides for contacts to compound semiconductors.

Device aspects ranged from near term issues in VLSI technology to novel structures such as metal based transistors, MIS structures with CaF_2 as the insulator, and amorphous Si phototransistors. The properties of contacts and interconnects for VLSI were reviewed by A. K. Sinha, and contributed papers addressed various topics related to materials for VLSI and packaging.

The wide range of topics presented in the symposium fostered broader understanding of the relationship of materials issues in several different technologies. We were pleased by the overall attendence of the symposium, and by the dedication of many attendees who were present from early Monday morning to late Friday afternoon.

Symposium Support: Defense Advanced Research Projects Agency (S. Roosild), Office of Naval Research (Electronics division, L. Cooper), Army Research Office (Materials division, J. Hurt), Hughes Aircraft Company, and Xerox Corporation.

Proceedings: Volume 54 of Materials Research Society Symposia Proceedings series.

Transport and Excitations in Polymers (Symposium F)

Symposium Organizers: T. Venkatesan, Bell Communications Research, Inc.; E. Kramer, Cornell University; R. H. Baughman, Allied Corporation

Diffusion in polymer melts of sufficiently long chains is believed to take place by reptation, a word coined by P. G. deGennes almost 15 years ago to describe the crawling of a chain along its own contour. Much of the discussion at the symposium on Transport and Excitation in Polymers focused on defining conditions necessary for reptations and other mechanisms that supercede it outside those limits. deGennes himself set the tone for the discussion with an excellent review of reptation and its relation to mutual diffusion. Nonlinear molecules, e.g., stars and rings, are of great interest as they should not diffuse by pure reptation. J. Klein and M. Rubinstein presented different theoretical models for the diffusion of stars and rings in linear matrices and rings in gels, respectively. Reports of experiments on stars diffusing in linear and crosslinked matrices (H. Sillescu), on stars in stars (B. Christ) and on rings in linear matrices (G. Hadziioannou) reveal a number of features not predicted by the models.

S. F. Edwards led off the afternoon session by describing a new theory of the glass transition using rigid rod polymers as a model system while M. Tirrell applied some of the previous ideas on reptation to describing the time dependence of the strength of polymer interfaces. A particularly interesting topic is the diffusion in polymer blends, where mass flows (Kirkendall effect) (S. Wu) and thermodynamic effects are particularly strong for polymers. In the latter case since the combinatorial entropy of mixing is almost negligible in polymer blends, segment interaction enthalpies should dominate the free energy of mixing and strongly enhance the mutual diffusion coefficient. Two papers (R. J. Composto et al. and R. A. L. Jones et al.) reported the first experimental evidence supporting the theory in separate blend systems.

A number of new techniques (or new wrinkles on old ones) were described for measuring the very small diffusion coefficients involved. The shear variety was impressive, from small angle neutron scattering (B. Christ) to forced Raleigh scattering (H. Yu, H. Sillescu) to NMR (E. D. von Merrwall) to fluorescence redistribution after photobleaching (B. A. Smith) to Rutherford backscattering spectrometry and forward recoil spectrometry (R. C. Lasky, R. J. Composto, G. Hadziioannou). Diffusion in polymer glasses occupied most of the second morning with an excellent lead-off review from H. B. Hopfenberg on the effects of physical aging on transport in glasses. Diffusion in glassy polymides was discussed for two quite different applications, electronic packaging (S. D. Senturia) and membranes for gas separation.

The chemistry, physics, and applications of polymeric metals and semiconductors provided another focus of the symposium. This section provided a combination of broad overview lectures for general audience and lectures describing the newest advances in materials synthesis and property understanding. The presentations provided a status summary from which a number of conclusions could be drawn.

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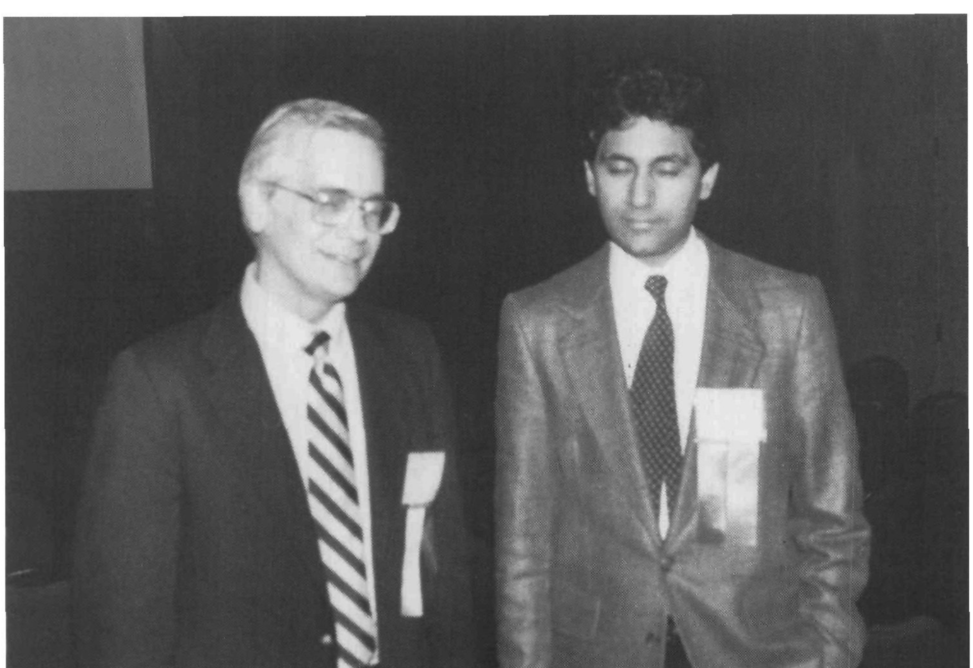
First, theoretical advances have provided reliable predictions of the electronic properties of single chains and have been successfully used to predict compositions that would be polymeric metals. However, there has been much less success in developing an understanding of interchain transport, and such transport appears to dominate conductivity. Also, much has been learned about the physics of carrier defects—solitons, polarons, and bipolarons. However, major refinements in theory are required to explain key details of the experimental results, such as the location of energy states in the gaps. Second, there has been an avalanche in the number of newly discovered conducting polymers, but, as yet, none of these compositions provides the complete property profile required for broad based applications. Conducting polymers are available which have desired conductivities, mechanical properties, stability, or processability, but no conducting polymers are known which combine all of these desired features. Finally, from the magnitude of interest and the pace at which important new discoveries are being made, it is clear that conducting polymers is still a rapidly evolving area with much for the future.

Another focus of the symposium was field-induced effects in polymers highlighted by invited lecturers on field induced switching in charge-transfer complexes, the nonlinear optical properties of conjugated polymers, piezoelectric polymers, and polymer electrets. The emphasis was (1) the optimization of field-induced effects via development of improved materials understanding and improved materials synthesis approaches and (2) device applications. Vladimir Dobrosavljevic, a graduate student in the Department of Physics at Brown University under Richard Stratt, received an MRS Graduate Student Award for his paper in this section on understanding the chromatic transitions of polydiacetylene solutions.

Different aspects of energy and excitation transport were covered in invited talks by C. W. Franks, S. Webber, and S. Etemad. An overview of photoconductivity in polymers was provided by P. M. Borsenberger. Polymers, being a class of weakly bonded solids, present unusual applications in the area of radiation-induced modification. Oblation of polymers by excimer laser pulses was reviewed by R. Srinivasan and there are interesting questions regarding the oblation mechanisms which are yet to be worked out. Applications of polymers to lithography was covered by G. N. Taylor and S. McDonald, and gas phase functionalization was proposed as an alternative to conventional wet developed resists. Synthesizing polymers for dry processing seems to be an important area of current research. There were several contributed and poster talks on radiation and particularly ion-beam effects on polymers.

G. Foti reviewed the radiation chemistry induced by ion irradiation of polymers, which seems to depend upon the ion species used. Several papers reported on ion-induced conductivity in polymers by ion irradiation, and for the first time, a pn junction was fabricated in a polymer (H. Sasabe). Clearly, this provides novel directions for ion-induced modification in polymers.



Symposium F Organizers (left to right): E. Kramer and T. Venkatesan.

Symposium Support: Army Research Office (Materials Science division) and Allied Corporation.

Cosponsor: Division of Polymer Chemistry, American Chemical Society.

Biomedical Materials (Symposium G)

Symposium Organizers: M. F. Nichols, University of Missouri; J. M. Williams, Oak Ridge National Laboratory; W. Zingg, University of Toronto

The Biomedical Materials Symposium at the Fall Meeting represented the first invitation by the core constituency of the Society to the biomaterials community to explore materials and techniques of common interest. Therefore program guidelines were designed to elicit information on a broad range of material problems, technologies and analysis techniques pertinent to bioengineering. Response of the biomaterial constituency to the interdisciplinary approach of MRS was enthusiastic. The symposium was generally regarded as one of the best that had been held in biomaterials.

Total attendance at all sessions was 450. It was estimated that 225 individual registrants, most of whom came primarily to attend the biomaterial symposium, were involved. This attendance was judged to be excellent in comparison with that of other forums in biomaterials.

Bioengineering practice varies more from one country to the next than does practice in many other technologies. The symposium was noteworthy for its international character in that important contributions were received from Canada, China, France, Germany, Sweden, Switzerland, and the U.K.

Needs required for further development of bioelectrodes were identified. Techniques such as reactive ion-beam etching, ion implantation for improvement of corrosion behavior or improved adhesion, various lithographic techniques and sputtering, all of which are traditionally of strong interest to MRS members, would appear to have much to offer in meeting microelectronics needs for bioelectrodes.

Orthopaedics comprises the largest market in biomaterials. A very strong program in this area included information on new materials, new processing techniques, and further assessment of existing practices.

At an informal wrap-up session it was concluded that in the future MRS will play an important role in disseminating information pertaining to biomaterials. This role will come about because the Society provides the conferences where information on the most advanced materials, processing techniques, and analytical techniques is exposed intensely and on a regular basis. At the same time, it was recognized that the Society must carefully define and

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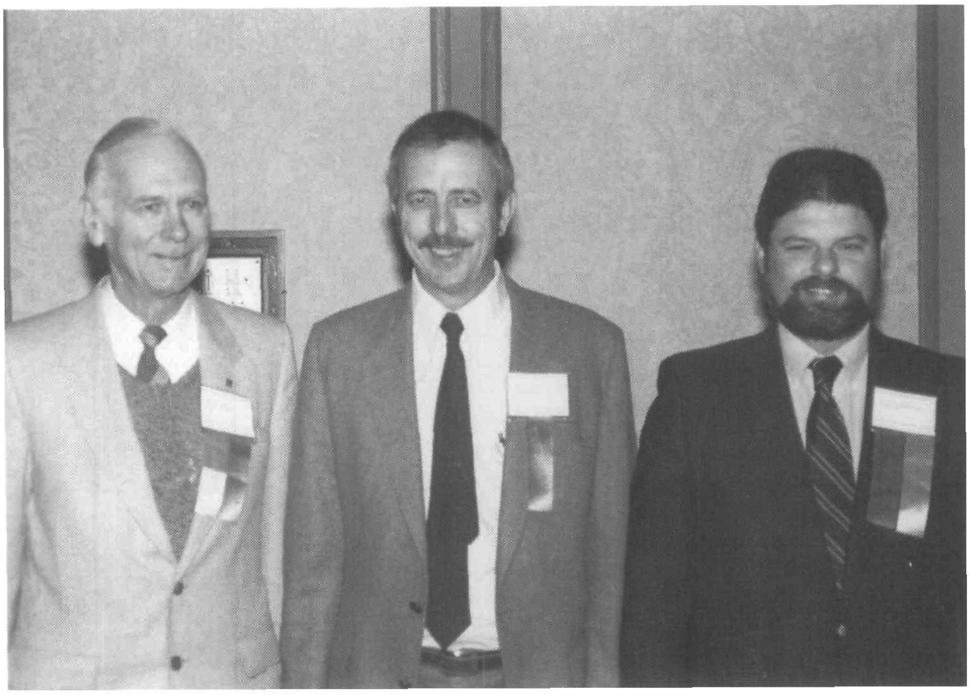

Symposium G Organizers (left to right): W. Zingg, J.M. Williams, and M.F. Nichols.

limit its role, so that its symposia will complement rather than duplicate an already crowded docket of conferences in biomaterials.

It was decided to hold the next major symposium on biomaterials at the 1988 MRS Fall Meeting. Topics to be featured are characterization of surfaces of biomaterials, characterization of the near-interface between tissue and materials, and surface treatments for biomaterials. Advanced techniques will be emphasized. Dr. Donald Ribbons of 3M expressed interest in serving as one of the organizers. Meanwhile, to help maintain continuity in the biomaterials area, the society is interested in entertaining proposals for a symposium of limited scope for the 1987 MRS Spring Meeting.

Symposium Support: Army Research Office, Materials Science Division; Howmedica; Johnson & Johnson Products, Inc.; National Science Foundation; Naval Medical Research & Development Command; Spire Corporation; U.S. Department of Energy; and Zimmer.

Proceedings: Volume 55 of Materials Research Society Symposia Proceedings Series.

Layered Structures and Epitaxy (Symposium H)

Symposium Organizers: J. M. Gibson, AT&T Bell Laboratories; G. C. Osbourn, Sandia National Laboratories; and R. M. Tromp, IBM Research Center.

The symposium Layered Structures and Epitaxy was the second MRS symposium on these topics and was quite successful. It was well attended, with nearly 100 oral and poster presentations. The four-day program contained sessions on epitaxial semiconductor films, surfaces and ultra-thin films, Schottky barriers and epitaxial silicides (combined sessions with Symposium E), quantum wells, strained-layer superlattices, Ge/Si and noncrystalline superlattices, and metal superlattices. The list of distinguished speakers included R. C. Pond, K. Takayanagi, E. J. van Loenen, G. A. Prinz, E. S. Yang, J. C. Hensel, R. T. Tung, P. S. Ho, L. L. Chang, P. Petroff, F. Capasso, J. N. Schulman, L. Dawson, T. Picraux, E. Kasper, E. Spiller, and T. Tsakalakos.

The interdisciplinary nature of this field was evidenced by the wide range of topics presented, including work on epitaxial growth, structural and electronic characterization, materials physics, and theoretical aspects of a large number of semiconductor, insulator, and metallic thin films and layered structures. This symposium provided a good forum for the exchange of ideas and different viewpoints in this area.

Symposium Support: Office of Naval Research, Air Force Office of Scientific Research, and High Voltage Engineering Europa B.V.

Proceedings: Volume 56 of Materials Research Society Symposia Proceedings series.

Phase Transitions in Condensed Systems (Symposium I)

Symposium Organizers: G. S. Cargill III, IBM Corporation; F. Spaepen, Harvard University; K. N. Tu, IBM Research Center

This two-day symposium was held in honor of Professor David Turnbull, on the occasion of his 70th birthday and his becoming professor emeritus at Harvard University. Several of Turnbull's students and associates, present and former, presented papers, as did others in the field. A total of four invited and 32 contributed papers was presented.

Continued

Symposium H Organizers (left to right): R.M. Tromp and J.M. Gibson.

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Following K. N. Tu's introduction to the occasion, G. S. Cargill gave an overview of David Turnbull's career and contributions, which he divided into four major categories, corresponding to the four sessions of the symposium: nucleation; liquids, glasses and glass formation; diffusion; and crystal growth. He also highlighted Turnbull's educational influence and his longtime co-editorship of the "Solid State Physics" series.

J. W. Cahn led off the nucleation session with an historical review of the emergence of modern nucleation theory. He pointed out how the work of Turnbull and collaborators in the late 1940s and early 1950s put the understanding of nucleation in condensed systems on a firm theoretical and experimental basis. That this work remains the foundation of the field even at this time was illustrated abundantly by the contributed papers on superheating of liquids and crystal nucleation in liquids and glasses, and martensitic nucleation.

Turnbull's unique role in the identification of the metallic glass state was reviewed by F. Spaepen. He noted how Turnbull had predicted the existence of the metallic glass state on the basis of his development, with M. H. Cohen, of the free volume theory for atomic transport in simple liquids, and of his demonstration of the attainability of large undercoolings in liquid metals. He went on to describe how, after Duwez's discovery that amorphous metals could be obtained by quenching of the melt, Turnbull and his student H. S. Chen were the first to demonstrate that these materials were indeed glasses, in that they exhibited the same physical manifestations of a glass transition as did the well-known silicate or organic glasses. Most of the contributed papers also dealt with metallic glasses, and provided an overview of the present understanding of the structure, formation and devitrification of these materials. Recent developments in the scattering techniques for studying the amorphous state, and in the synthesis of oxide glasses were also presented.

D. Lazarus presented a review of the present understanding of atomic diffusion in crystalline and amorphous metals. He highlighted Turnbull's contributions to this field: the first measurements of grain boundary diffusion, the identification of the mechanisms for fast diffusion of transition and noble metals in semiconductors and polyvalent metals, and the study of diffusion in amorphous metals. Several diffusion-related phenomena were presented in the contributed papers: direct observation of surface diffusion, diffusion in multilayered semiconductors, interface structure and diffusion, precipitation and ordering, and formation of amorphous metals by interdiffusion of the crystalline elements.

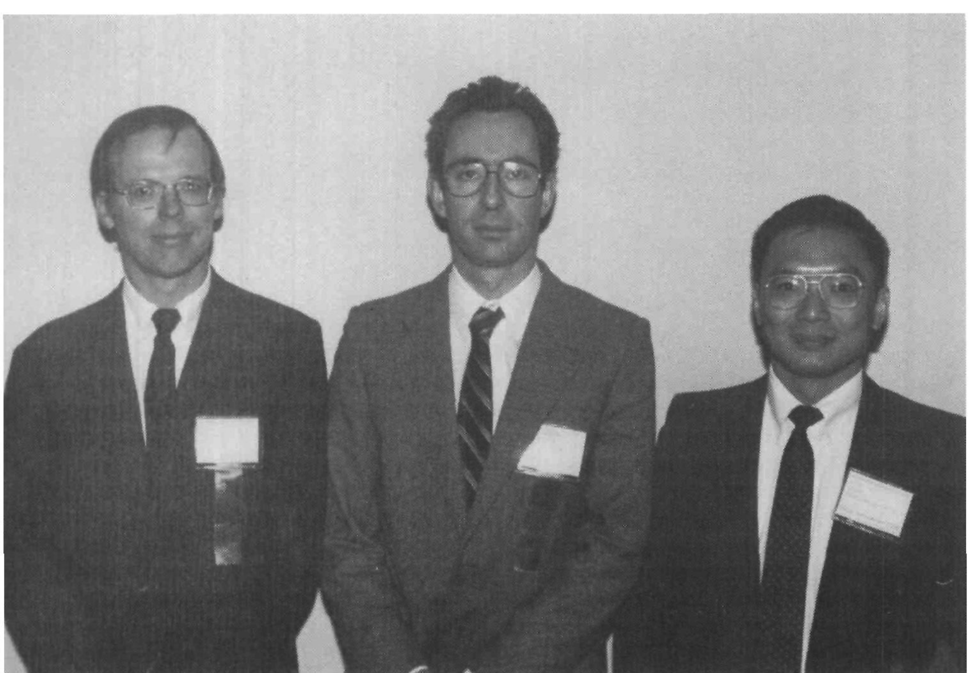
The contributions of Turnbull and coworkers to the understanding of crystal growth were reviewed by M. E. Glicksman. Among them were his work on faceted growth, the demonstration of crystal growth-melting symmetry in some oxide systems, the discovery of the enhancement of crystal growth in open structures by the application of pressure, and, most recently, his analysis of the very fast crystallization processes accompanying pulsed laser quenching. The contributed papers covered an interesting diversity of phenomena and materials: formation of liquid crystals, quasicrystals and two-dimensional phases, melting of amorphous silicon, solute trapping, secondary grain growth, and precipitation.

David Turnbull (center) attends Symposium I, held in his honor.

On the evening of the first day, a dinner in David Turnbull's honor was held at the Cronkhite Graduate Center at Harvard. It was attended by 125 of his friends, many of whom had come specifically for the occasion. The after-dinner speech by M. H. Cohen included a personal reminiscence about Turnbull's career, their association, and the evolution of the scientific environment over the last 40 years.

Symposium Support: Allied Chemical Corporation, Energy Conversion Devices, Exxon Research and Engineering Company, General Electric Company, and IBM.

Proceedings: Volume 57 of Materials Research Society Symposia Proceedings series.



Symposium I Organizers (left to right): G.S. Cargill III, F. Spaepen, and K.N. Tu.

Rapidly Solidified Alloys and Their Mechanical and Magnetic Properties (Symposium J)

Symposium Organizers: B. C. Giessen, Northeastern University; D. E. Polk, Office of Naval Research; A. I. Taub, G. E. Corporate Research and Development

This symposium was the third in a biannual series on rapidly solidified materials and their properties held by MRS (1981, MRS Symposia Proceedings Volume 8 and 1983, MRS Symposia Proceedings Volume 28). Like its predecessors, it consisted of five oral presentation sessions and a large poster session; the latter accommodated eight late papers and was open up

Continued

Symposium J Organizers (left to right): B.C. Giessen, D.E. Polk, and A.E. Taub.

to the time of the conference. The symposium drew strong international response from Britain, Canada, China, France, Germany, Sweden and especially Japan.

The first two sessions dealt with fundamentals, the structure and properties of several types of metastable phases and processing techniques. Concerning glass formation, W. L. Johnson (Caltech), reviewed the principles underlying glass formation by diffusion in the solid state which had been pioneered by his group. R. Hasegawa (Allied Corporation) reviewed relations of electronic structure and glass formation. The status of electronic structure calculations on glassy metals was discussed by D. M. Nicholson (University of Tennessee). A substantial group of papers dealt with a recently discovered new class of solids, the quasiperiodic crystalline materials. Their formation, especially in the Al-Mn system, was reviewed by R. J. Schaefer (NBS). Papers were presented on their structure, occurrence in several new alloy systems, formation by pulsed electron beam surface melting, thermal properties, and theoretical interpretation in terms of fractals. Of special interest were data on the partially periodic, partially quasiperiodic T phase presented by L. Bendersky (NBS). Other fundamental papers dealt with compositionally modulated thin films, discussed by T. Mizoguchi (Gakushuin University), catalytic properties of transition metal alloy glasses and relaxation phenomena.

Papers on processing showed the great strides being made in bringing improved rapid solidification techniques to maturity for industrial processing. B. L. Mordike, (University of Clausthal, Germany), reviewed the state of the art of laser processing of materials; high-power laser surface treatment involving surface melting, alloying, and cladding is now moving from laboratory to commercial application. Other processes analyzed in detail included the double roller method (F. Kogiku et al., Kawasaki Steel Corporation) and thin film sputtering methods (M. Naoe, Tokyo Institute of Technology). The latter were treated further in other papers (see below). Changes in solidification morphology during rapid freezing were discussed by V. Laxmanan (NASA).

Two full sessions were devoted to the mechanical properties of rapid solidification materials. The papers covered the advances obtained in Co, Al, Fe, Mg, Ni, and Ti alloys processed by atomization, laser surface treatment, melt spinning, melt extraction, explosive consolidation, and dynamic liquid compaction. The progress in Al alloys reviewed by J. R. Pickens (Martin Marietta Laboratories) can be divided into several areas. Improvements in the ductility of the low density, high modulus Al-Li alloys have been obtained by rapid solidification processing, but in his review Pickens predicted stiff competition from the newly developed ingot metallurgy alloys. Other papers discussed high-temperature Al alloys, including Al-rare earths and Al-Fe-V alloys. The latter alloy, discussed by D. Raybould (Allied Corporation), is produced at Allied's melt spinning facilities which incorporate in-line pulverization to reduce contamination.

H. Jones (Sheffield University) reviewed the advances in Mg alloys, pointing to areas with potential for future advancements. The challenges in these alloys include promotion of non-basal slip, creation of metastable cubic phases and strengthening of high temperature Mg-base intermetallics. For nickel-base alloys, rapid solification has produced increased ductility of intermetallic compounds as reviewed by A. I. Taub (General Electric Corporation), refined microstructure of superalloys, and superplastic flow at high temperature. The largest grouping of papers concerned Ti alloys, led off by the review of F. H. Froes (AFWAL). Improved properties of Ti and Ti_4Al-base alloys through the introduction of fine dispersoids was discussed by several authors, including R. G. Rowe (General Electric), A. G. Jackson (Systems Research Laboratory, Inc.) and S. H. Whang (Northeastern University). In consolidated specimens of melt-extracted Ti alloys, the dispersoids were shown to retard grain coarsening and improve post-creep tensile ductility. Wear properties of consolidated rapid solidification alloys were discussed by T. Vreeland, Jr. (Caltech).

Although this group of papers covered a wide range of alloy classes, several common approaches to improving mechanical behavior by rapid solidification processing were evident including laser surface treatment, spray forming and devitrification of amorphous alloy precursors. Interest in the latter also extended to the mechanical properties of the glassy phase, particularly annealing embrittlement.

The session on magnetic behavior addressed a wide range of topics. R. C. O'Handley (MIT) reviewed current views on the correlations between magnetic properties and structural changes in amorphous alloys. The hysteresis loop observed in the temperature dependence of the magnetization, magnetostriction, etc. of amorphous Co-Nb-B alloys is ascribed to a reversible transformation in the local short range order. A. Collins (MIT) studied the relationship between the magnetic aftereffect and the magnetostriction of a series of amorphous Fe-Cr-B and Fe-Nb-B alloys. D.Raybould (AlliedCorporation) discussed the production of thicker amorphous metal strip from the thinner ribbons formed by planar flow casting by the application of pressure and heat. Localized bonding between the ribbons appear to be due to a silicon oxide based film which also electrically insulates the ribbons from each other.

G. S. Canright (ORNL) discussed the effect of Ce on the annealing behavior of Fe-based amorphous metals. Addition of 75

Continued

ppm Ce prevents embrittlement of $Fe_{80}B_{16}Si_2C_2$ upon annealing up to the onset of crystallization. A similar effect was found in $Fe_{80}B_{20}$, but not in $Fe_{78}B_{13}Si_9$. The Ce addition also reduced quenched-in stressed, as demonstrated by the elimination of maze domains. It was suggested that Ce substantially affects the diffusion rates and hence stress relief rates in the alloy, possibly via interactions with impurities such as O and S.

Presentations by G. C. Hadjipanayis (Kansas State University) and K. V. Rao (Royal Institute of Technology, Stockholm) focused on the microstructure and hard magnetic behavior of rapid quenched iron-rare-earth-metalloid crystalline alloys, in particular the alloys containing $Fe_{14}Nd_2B$ which have outstanding hard magnetic properties. Y. Niimura(Tokyo Institute of Technology) described the "Targets Facing" sputtering technique where in two targets face each other with the magnetic field and plasma confined between them. The substrate is placed outside of the plasma so that only neutral atoms arrive; this arrangement also allows the use of very low Ar pressure, e.g., 1 mtorr. Unlike the columnar Co-Cr films resulting from conventional sputtering, a much finer cellular structure is obtained.

In view of the success of this symposium series, a related symposium is planned by MRS for the 1986 Fall Meeting, to be arranged by W. Johnson (Caltech), L. Tanner (Lawrence Livermore National Laboratory) and M. Tenhover (SOHIO).

Symposium Support: Allied Corporation, General Electric Company, Martin Marietta Laboratories, and Pratt and Whitney Aircraft.

Proceedings: Volume 58 of the Materials Research Society Symposia Proceedings series.

Oxygen, Carbon, Hydrogen, and Nitrogen in Silicon
(Symposium K)

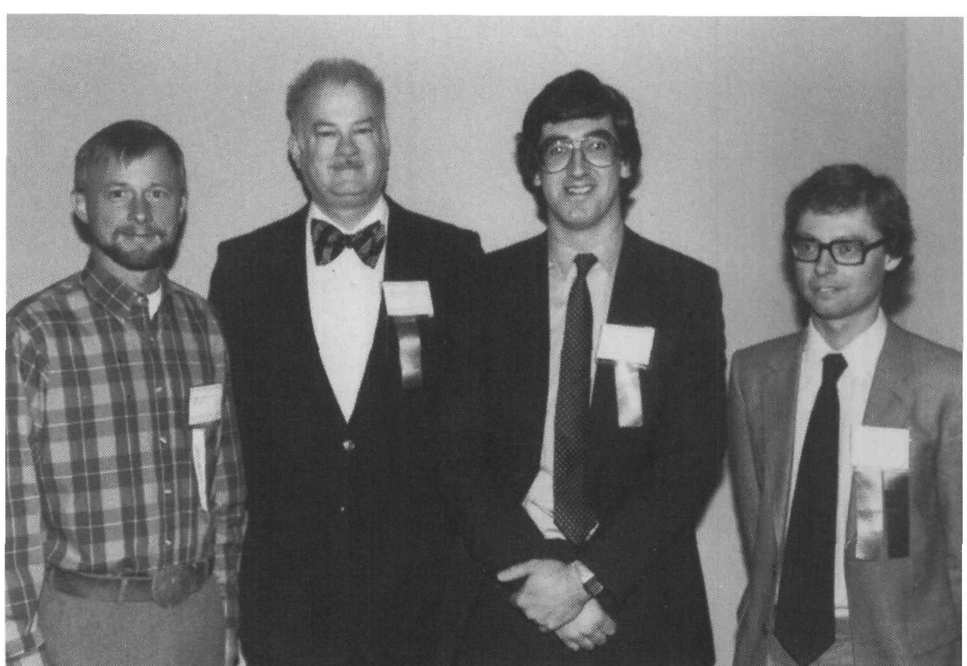
Symposium Organizers: J. W. Corbett, State University of New York; J. C. Mikkelsen, Jr., Xerox Palo Alto Research Center; S. J. Pearton, AT&T Bell Laboratories; S. J. Pennycook, Oak Ridge National Laboratory

This symposium reviewed the state of understanding of the technologically important light-element impurities in silicon, namely oxygen, carbon, hydrogen and nitrogen. A feature of the review presentations was the recognition that these impurities may be interactive under certain conditions, and that a variety of experimental techniques must be utilized to explore their behavior in the silicon lattice. A total of 18 invited papers, 28 orally presented contributed papers, and 21 contributed poster papers were presented during the symposium.

Three sessions were devoted specifically to oxygen in silicon. In the first, chaired by J. R. Patel (AT&T Bell Laboratories), the characteristics of oxygen precipitation were examined. A. Bourret (CEN, France) presented a detailed high-resolution transmission electron microscopy (HRTEM) study of the evolution of oxygen-containing clusters as a function of thermal treatment. The ability of HRTEM to distinguish different phases of SiO_2 precipitates by direct inspection of their lattice structure represents an exciting and pivotal development in the understanding of oxygen clustering phenomena. T. Y. Tan (IBM) and S. M. Hu (IBM) each presented detailed microscopic models on different aspects of SiO_2 precipitate formation and growth. The importance of the role of lattice defects, in particular Si interstitials, in determining the kinetics of these processes was emphasized.

The second session on oxygen, chaired by J. W. Corbett (SUNY-Albany) was devoted to an intense discussion of the nature of the various thermal donors induced in silicon by annealing of Czochralski grown silicon at low-to-moderate temperatures. L. C. Kimerling (AT&T Bell Laboratories) presented an overview on the properties of the 450°C donors and the accumulated evidence for their possible structure. M. Stavola (AT&T Bell Laboratories) reviewed the experiments leading to an understanding of the electronic structure and atomic symmetry of these same donors, while J.-M. Spaeth (University Paderborn, West Germany) presented data from recent magnetic resonance experiments on the nature of the donor core. The optical properties and evolution of the donor characteristics with annealing time at 450° C were detailed by P. Wagner (Heliotronic, West Germany), showing the presence of at least eight different donor states which apparently grow from the same core structure. Various models for this core, obtained by quantum mechanical cluster calculations, were presented by L. C. Snyder (SUNY-Albany). The interrelationship with the previous session was obvious because oxygen donor formation is an early state of oxygen clustering and precipitation.

The third session devoted to oxygen in silicon was chaired by W. Lin (AT&T Bell Laboratories) and dealt with bulk oxygen behavior and related defects. J. C. Mikkelsen (Xerox PARC) reviewed the solubility and diffusivity data for oxygen, and presented results from high-temperature mass transport and low-temperature reorientation experiments revealing the intrinsic diffusion of oxygen to be described by a single relationship over the entire temperature range. The intrinsic effects which may enhance this rate were also described. J. L. Lindstrom (University Linkoping, Sweden) presented an overview of the oxygen-defect related complexes in silicon and their evolution with annealing. A topic which combines many of the previously mentioned topics is the gettering of deep-level, metal-related impurities in silicon by various intrinsic or extrinsic methods. A. Ourmazd (AT&T Bell Laboratories) reviewed the possible mechanisms for this technologically crucial phenomenon, using both HRTEM and secondary ion mass spectrometry (SIMS) to better understand the complex interplay between defect



Symposium K Organizers (left to right): J.C. Mikkelsen Jr., J.W. Corbett, S.J. Pearton, and S.J. Pennycook.

diffusion, solubility and trapping. K. Sumino detailed the possible interactions of impurities with dislocations in silicon, a topic of related interest.

The effects of even < ppma carbon concentrations in silicon are being increasingly noticed as circuit manufacturers strive for even higher performance levels and smaller device dimensions. The symposium session, chaired by G. Davies (Kings College, London) was highlighted by a review of the properties of carbon in silicon by R. C. Newman (University of Reading, U.K.) in which analysis techniques for carbon, the solubility and diffusivity of the element, and its interaction with other impurities and with defects were described. U. Gosele (Duke University) reviewed the role of carbon and point defects in silicon, in, for example, enhancing SiO_2 precipitate formation.

R. N. Hall (General Electric Company) chaired the session on hydrogen in silicon. Hydrogen is important because of its ability to passivate electrically active bulk and surface defects or impurities in all forms of silicon, and is an important component in plasmas used for the dry etching of small features in SiO_2 dielectric layers. S. J. Pearton (AT&T Bell Laboratories) presented an overview of the properties of hydrogen in silicon, dealing with the passivation by atomic hydrogen of deep and shallow level impurities, and the diffusivity and solubility of the various states of hydrogen.

Nitrogen is an increasingly important impurity in silicon because of its ability to harden the lattice. S. J. Pennycook (ORNL) and G. D. Watkins (Lehigh University) chaired a session highlighted by talks from T. Abe (SEH, Japan) and H. J. Stein (Sandia National Laboratories) reviewing the nature of nitrogen-related defects in silicon, the solubility and diffusivity of nitrogen, and the possible aggregation phenomena occurring between nitrogen atoms and other impurities or defects in silicon. R. J. Jaccodine (LehighUniversity) presented an invited talk on nitridation-induced reactions on silicon surfaces, an exciting area of development as the search for improved dielectric layers continues. The complex surface chemistry occurring during nitridation by various techniques was outlined and specific models for this process discussed.

An extremely successful poster session provoking a good deal of interactive participation was held on Thursday evening of the MRS Fall Meeting. The dominant theme of the session was clearly oxygen precipitation phenomena, ranging from thermal donor formation to high temperature phases of SiO_2.

The technological importance of the symposium content was clearly seen in the high level of sponsor support, and the essentially equal participation of attendees from university and industry emphasized the interplay of fundamental studies with technological applications. The international nature of the symposium, evidenced by the high level of overseas speaker participation, also reflected an appreciation of the understanding of the importance of oxygen, carbon, hydrogen, and nitrogen in silicon.

Symposium Support: ARCO Solar Inc., Cabot Corporation, Department of Energy, Exxon Corporation, General Electric, Hughes Aircraft Company, Jet Propulsion Laboratory, Mobil Solar Energy Corporation, Monsanto Electronic Materials Company, Rockwell International, Rome Air Development Center, (Solid State Science Division), SEH America, Inc., Solarex, and Wacker.

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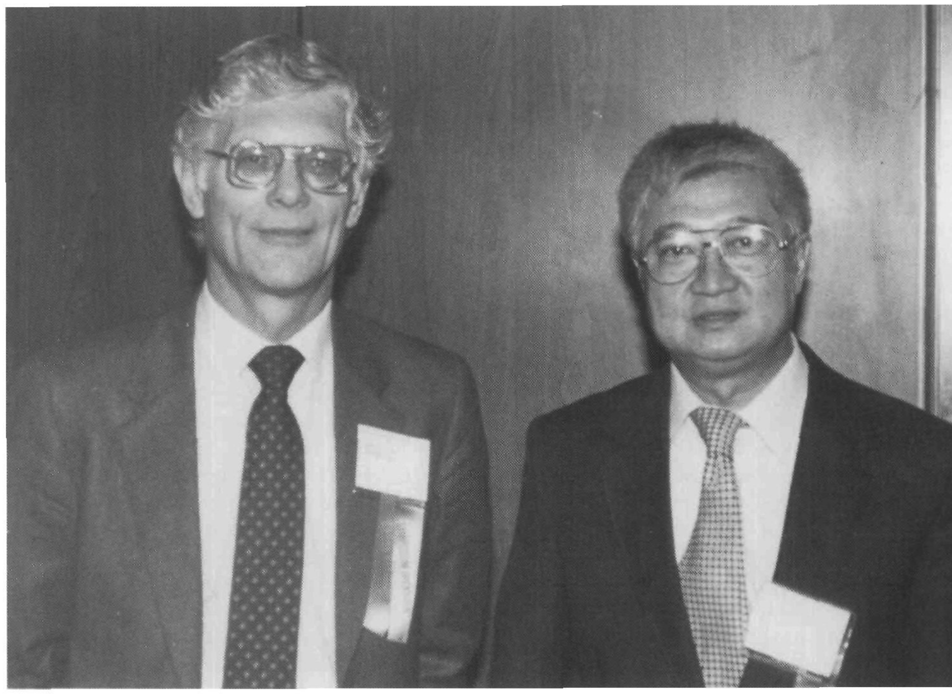

Symposium L Organizers (left to right): R.J. Stokes and Y. Chen.

Defect Properties and Processing of High-Technology Nonmetallic Materials (Symposium L)

Symposium Organizers: Y. Chen, Oak Ridge National Laboratory; W. D. Kingery, Massachusetts Institute of Technology; R. J. Stokes; Honeywell, Incorporated

Symposium L on Defect Properties and Processing of High-Technology Nonmetallic Materials was the second in a series to be held every other year. It reviewed some of the exciting progress taking place in advanced ceramics, particularly in physical properties and ceramics processing. The symposium opened with an overview of the report of the Research Briefing Panel on Ceramics and Ceramic Composites by J. B. Wachtman. The overview stressed the advantages to be gained right now through imaginative design of ceramics and in the future through design of ceramics, which will establish competitive positions for both electronic and structural applications.

Many of the papers dealt with the synthesis of ceramics through novel chemical routes. Ceramic powders of exceptional purity may be synthesized through vapor phase reactions induced by laser or plasma heating or by precipitation from chemical solutions. F. F. Lange pointed to the advantages gained through knowledge of colloid chemistry in the control of dispersion, sedimentation, and flocculation of these powders prior to additions for doctor blading or slip casting of the green, prefixed, ceramic. He and others cautioned that preserving these advantages requires great care in avoiding agglomeration or organic contaminants which can later originate flaws in the bulk material. In some cases ultra-clean room techniques have been employed to maintain the purity through to the finished material. R. Roy reminded us of the long history of sol-gel chemistry and its use in the preparation of both homogeneous and heterogeneous (diphasic) high-purity starting material.

Insight into the origins of flaws during sintering was presented by A. G. Evans, who showed that differential densification results in hydrostatic stresses. He pleaded for a better fundamental understanding of the sintering of heterogeneous systems

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which is essential for the successful fabrication of composites. M. P. Harmer showed how additives sensitivity affect the final microstructure of sintered electronic ceramics. Novel thermal processing of materials using the principles of specific and selective heating of materials by microwaves at 2.45 GHz was covered in detail. W. Tinga presented the general energetics of microwave heating with application to ceramics. V. K. Varadan gave an outstanding paper on the radiation-material interaction based on the isomeric parity of coiled organic polymers. This model shows promise for understanding the interaction of microwaves with general organic materials.

J. Narayan discussed laser and ion-beam mixing of metal overlayers in insulators, and in particular SiC and Si_3N_4. These surface modification techniques were shown to have an effect on physical and mechanical properties of these materials. The fracture toughness of laser treated SiC were shown to improve.

There was much emphasis on thin film ceramic preparation through either the controlled decomposition of thin layers of metallo-organic, sol-gel or polymeric precursors, or the direct deposition by sputtering or chemical vapor deposition techniques. These techniques have a number of advantages: they can be low temperature, they produce materials with a very fine grain size (100Å), and the compositions can be tailored for specific applications.

H. K. Bowen reviewed the economic aspects of alternative ceramic processing techniques. He stressed that while modern chemical approaches involve costly starting materials the processing is cheaper and improved yield is most critical in the future economic advantages of the chemical route to ceramic fabrication.

Many papers highlighted new insights into improved fundamental understanding of the physics and chemistry of bulk phenomena. J. H. Harding and C. R. A. Catlow showed how recent expansion of pair-potential methods to handle larger systems (supercells) resulted in accurate theoretical descriptions of both the lattice thermal expansion of calcium fluoride and an explanation for the changing coordination with temperature of yttrium as revealed by EXAFS studies on yttria-stabilized zirconia. The detailed chemistry of point defects and their dependence on dopant concentration, temperature, and oxygen partial pressure received much attention. Authors showed how the chemistry is critical to the understanding of transport phenomena underlying many physical properties such as ionic conductivity, thermoelectric power, radiation damage, and the stability during annealing of important electronic, optical, and electro-optic materials.

Structural defects such as dislocations and grain boundaries can significantly affect the physical behavior of nonmetallic materials. Sophisticated TEM analysis of dislocations, stacking faults and grain boundaries by C. B. Carter and others showed how detailed atomic arrangements are affected by ionic and covalent bond character and ionic differential in ceramic materials. The electronic band structure in the vicinity of grain boundaries in particular affects the charge transfer across the interfaces and the characteristics of capacitors and varistors as a consquence.

The symposium also focused on the optical and mechanical behavior of nonmetallic materials. R. C. Powell and others described the fluorescence characteristics of active ions placed in laser host crystals. Subtle effects of lattice site location and environment affect the conversion efficiency. Examples were given of improvements in laser operation in alexandrite, titanium-doped sapphire, YAG, and β''-alumina hosts through better control of the solid-state chemistry. The fabrication of optical wave guides either in the form of optical fibers or surface channeled devices was reviewed. T. Miyashita described the tremendous progress made in the reduction of loss through purification and process improvements in silica, fluoride, and chalcogenide fibers for the visible and infrared spectral range. R. Holman and others presented the essential technical requirements for guided wave integrated optics produced by titanium diffusion or implantation into lithium niobate. Crystal perfection, purity, thermal stability during diffusion or implantation anneals, the ability to place electrodes were cited as essential to the successful device implementation.

The significant increases in mechanical strength and fracture toughness in zirconia-based ceramics were reviewed by A. H. Heuer. Reasons for the improved mechanical properties originate in microstructure and grain size control and the toughening associated with the structural phase transformations in zirconia. This class of ceramics has now evolved to the point where it can be regarded as flaw size insensitive. The search for alternative systems exhibiting a martensite phase transformation is attractive.

The symposium was well attended throughout, reflecting the considerable interest in advanced ceramic materials. The topics covered were broad in range and the treatments varied from the very fundamental to the pragmatic.

Symposium Support: Defense Advanced Research Projects Agency, U. S. Department of Energy, and Honeywell, Inc.

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Oxides, Zeolites, and Clays in Catalysis (Symposium M)

Symposium Organizers: D. E. W. Vaughan, Exxon Research and Engineering Company, A. W. Sleight, E. I. du Pont de Nemours

This symposium comprised 30 papers over three days, with a day devoted to each of the three program segments—oxides, zeolites and clays. Most of the papers

Continued

Symposium M Organizers (left to right): D.E.W. Vaughan and A. Sleight.

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reported new material, many of which are either "in press" or about to be published. The presentations were well attended throughout, reflecting the interest of the subject matter to both the established MRS membership, and new members primarily attending this symposium.

The opening lecture by J. M. Thomas (Cambridge University) reviewed strategies for characterizing new mixed oxides and microporous, microcrystalline materials, overviewing all the subject materials of the meeting. The first Oxide session on "Catalyst Characterization" commenced with an invited paper by F. S. Stone (Bath University) on the characterization of basic oxides used as catalysts, matrices, and supports; and the afternoon session with an invited talk by J. H. Lunsford (Texas A&M University) on the solid-state chemistry of methane oxidation catalysts (coauthored by J-X. Wang). Other papers on oxides were presented by I. Wachs (Exxon), J. Bradzil (Sohio), B. Davis (University of Kentucky), A. Ferretti (DuPont) and J. Lennhoff (Worcester Polytechnic Institute).

The day on Zeolites was divided into sessions on "Zeolite Synthesis and Characterization" and "Zeolite Structural and Catalytic Characterization." The invited talk in the first of these was given by D. E. W. Vaughan (Exxon), covering trends and developments in zeolite science, and the second by D. Barthomeuf (Université Paris) discussed zeolite acidity, with emphasis on the influence of the structural and chemical environment. Other papers on zeolites were presented by R. Szostak (Georgia Tech), A. Chester (Mobil), G. Skeels (Union Carbide), R. Gorte (University of Pennsylvania), C. Catlow (London University), W. Rohrbaugh (Mobil), R. Shannon (DuPont), R. Czencsits (Lawrence Berkeley Laboratory), D. Vaughan (Exxon), and E. Oldfield (University of Illinois).

The third of the main subject groups, Clays, included both pillared clays and sheet hydroxides. The invited lecture in the session on "Synthesis and Characterization of Clays and Pillared Clays" was presented by J. J. Fripiat (CNRS, Orleans), discussing the formation mechanism, structure and surface properties of pillared (Al_{13}) beidellite (coauthored by A. Schultz, G. Poncelet, and W. Stone). The rest of this session focused on the sheet hydroxides, with papers by W. Reichle (Union Carbide), P. Biloen (University of Pittsburgh), and T. Pinnavaia (Michigan State University). The session "Clay and Pillared Clay Catalysts" began with an invited talk by R. A. van Santen (Shell) detailing the hydroisomerization activity of nickel substituted montmorillonite. This session was completed with papers by M. Occelli (Gulf Oil), F. Fitch (Laporte), S. Komarneni (Pennsylvania State University), U. Chowdhry (DuPont), and D. Vaughan (Exxon).

Symposium N Organizers (left to right): D.E. Passoja, B.B. Mandelbrot, and R. Laibowitz.

Symposium Support: International Zeolite Association, Exxon Research and Engineering Company, E. I. du Pont de Nemours & Company, Air Products and Chemicals, Amoco Corporation, Engelhard Corporation, Standard Oil Company (Ohio).

Fractal Aspects of Materials (Symposium N)

Symposium Organizers: R. B. Laibowitz, IBM Research Center; B. B. Mandelbrot, Harvard University; D. E. Passoja, Passoja Incorporated

The increasing interest in fractals within the scientific community was reflected in the strong growth of the fractals symposium over last year. The three-day symposium at the Fall Meeting also included a Tuesday evening poster and discussion session. Fractal geometry is becoming a widely used tool for the analysis and characterization of materials and for modeling of static and dynamic transport properties. The symposium attracted great attention since it also dealt with many specialized applications of fractals within materials science and basic physical processes.

This year the symposium began with two tutorial talks. R. Voss gave a visual introduction to fractal shapes and reviewed the mathematical definitions and experimental measurement techniques for estimating the fractal dimension. D. Schaefer presented a step-by-step illustration of the use of fractals in characterizing various stages of the aggregation processes and discussed the use of scattering measurements for determining fractal properties.

Variations of the aggregation process have all been interpreted in terms of fractals. D. Weitz, A. Hurd, J. Wilcoxon, G. Gollub, and D. Ensor presented experimental data on various aggregating systems. L. Sander and R. Messier discussed theoretical concerns of ballistic aggregation while H. Wiesmann discussed Laplacian fractals as a generalized model for diffusion limited aggregation and dielectric breakdown.

Behavior and time dependence at fractal interfaces were considered by many authors, e.g., B. Sapoval, J. P. Champigny, T. Kaplan, R. Corderman, and M. Keddam. In addition, other dynamic properties of fractal materials were presented by J. Klafter (relaxation), R. Kopelman (exiton kinetics), S. Tam (random walks), J. Drake (diffusion and reaction), and Y. Gefen (transport in metallic networks).

Several interesting papers on mechanical properties and fracture in materials were presented. The work of Y. Termonia, M. Ausloos, E. Louis, and J. Mecholsky dealt with the fractal nature of actual fractures. K. Sreenivasan presented some of the fractal aspects of turbulence. P. deGennes discussed the expected large influence of fractal pore geometry during the wetting process.

Many papers emphasized the more theoretical aspects of the application of fractal concepts to materials problems. R. Orbach discussed how the high-frequency vibrational modes in fractal materials (fractons) influence physical properties and suggested that most amorphous and disordered materials are actually fractal at small scales. B. Mandelbrot, the inventor of fractals and one of the symposium organizers, presented

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new results on self-affine (as opposed to the more common self-similar) fractals. Scattering calculations from fractals were presented by P. Schmidt. Additional theoretical and practical insight was provided by presentations dealing with rough surfaces by F. Family and M. Kardar. Several workers presented fractal characterizations of various materials from microscopic to geological distance scales. Small metal particles, ore deposits, engineering surfaces, dust grains, fractally layered superconducting films, naturally occurring gold particles and fractal scaling in brain protein were among the many interesting materials presentations.

Symposium Support: E. I. du Pont de Nemours and Company, Inc., Exxon Research and Engineering Company, IBM T. J. Watson Research Center, and Office of Naval Research.

Extended Abstracts: Published by MRS as Vol. EA-6.

Nonlinear Optical Materials (Symposium O)

Symposium Organizers: A. M. Glass, AT&T Bell Laboratories; D. A. B. Miller, AT&T Bell Laboratories; C. L. Tang, Cornell University

The symposium on Nonlinear Optical Materials was conceived as a forum for the exchange of views among the diverse range of workers in the field of nonlinear optics in a way not normally covered by other conferences in the field. Since much of the practical usefulness of nonlinear optics depends critically on the ability to fabricate suitable materials and to understand their properties, it is important that workers in the physics of nonlinear optical properties, in the growth of suitable materials, and in the invention and development of new devices and applications should exchange information. Consequently, the program for this symposium was particularly broad.

The first session, on polymer materials, opened with an invited talk by A. F. Garito who summarized the nonlinear optical properties and growth of polymers. Other papers in the session dealt with properties and growth of polydiacetylenes and glassy polymer films. An invited paper by R. S. Hellwarth started the following session on photorefractive materials. He discussed optical measurements of impurities and drift and diffusion in bismuth silicon oxide and barium titanate crystals. Deep levels in bismuth germanium oxide, general properties of tungsten bronze crystals, characterization of strontium barium niobate, and tensor photovoltaic effects were discussed by other contributors.

The sessions on semiconductors and microstructures included an invited talk by A. C. Gossard, who reviewed the growth and nonlinear optical properties of quantum well structures. Contributed papers covered excitonic absorption saturation in GaAs, InGaAs and ZnMnSe quantum wells as well as theoretical work on quantum well nonlinear properties. Other topics covered included large nonlinear optical responses from CdS excitonic effects, ultrafast saturation effects in GaAs, two photon absorption in various materials and thermal effects in ZnSe. C. Flytzanis presented an invited paper on the nonlinearities of composite materials including metal colloids and semiconductor doped glasses.

In the session on organics, I. Ledoux gave an invited paper on molecular organic crystals, both in bulk and in wave guides. Laser-induced deposition of organic materials, growth of urea crystals and harmonic generation in crystal-cored fibers were also discussed. R. L. Byer reviewed work on a large number of materials and techniques in an invited talk that opened the session on inorganic materials. Other papers dealt with flux growth of KTP, characterization of lithium niobate, and frequency mixing using lithium niobate with periodic domains. A post deadline paper presented calculations of second-order polarizabilities.

B. G. Kushner presented an invited overview of DOD requirements for nonlinear optical materials in the session on applications and growth. In another invited talk, W. C. Egbert described growth of nonlinear crystals in space. Other papers described the use of nonlinear optics for characterizing semiconductor surfaces, and measurements of nonlinear properties of liquid crystals. The final session opened with an invited talk by Chen Chuangtian on the second-order nonlinearities of boron-oxygen compounds. Contributed papers included discussions of organic molecule nonlinearities, measurements of third order nonlinearities in transparent media, optimization of acoustoroptic materials, and nonlinearities in biphenyl and ethynbenzene derivatives.

Symposium Support: Defense Advanced Research Projects Agency (J. Neff).

Extended Abstracts: Extended Abstracts Volume EA-7.

Symposium O Organizers (left to right): D.A.B. Miller and C.L. Tang.

Defects in Glasses (Symposium P)

Symposium Organizers: Frank L. Galeener, Xerox Palo Alto Research Center; David L. Griscom, Naval Research Laboratory; Marvin J. Weber, Lawrence Livermore National Laboratory

The symposium on Defects in Glasses reviewed numerous advances which have been achieved over the last several years in our conceptual and quantitative understanding of imperfections in amorphous insulators and chalcogenide semiconductors. Eleven invited talks and 26 contributed papers were grouped into 10 topical sessions.

Two of the best attended sessions were devoted to defects in the amorphous forms of silicon dioxide. The majority of the papers in this grouping dealt with electron spin resonance (ESR) characterizations of paramagnetic point defects and the theoretical modeling of these. It was evident that the theoretical contributions have assumed an increasingly important role in interpreting the ESR spectra. Materials systems investigated included pure bulk

Continued

Symposium P Organizers (left to right): D.L. Griscom, M.J. Weber, and F.L. Galeener.

synthetic silicas, thermally grown thin films, and germanium-doped silicas produced by chemical vapor deposition or sol-gel processes. Surprisingly, the emphasis was almost equally divided between defects produced in the traditional way by ionizing radiation and defects induced by sub bandgap laser light. Particularly striking was a report of volume compactions of up to 36% being accomplished in thermal SiO_2 films by ultraviolet irradiation. Another paper found that preirradiation with gamma rays can lower the threshold for laser induced breakdown in bulk silica.

Chalcogenides also claimed two sessions, one of which emphasized the subject of intermediate range order, principally in glassy Si_xSe_{1-x}. Raman spectroscopy, EXAFS, neutron diffraction, and melt viscosity were the main experimental probes in the latter materials. The data indicated significant differences between the structures of crystalline $SiSe_2$ and the glasses in the range $SiSe_2$ to Si_2Se_3. A crosslinked chain cluster model was proposed for the vitreous forms. The ability to form glasses in the system $(Ge_{1-y}Sn_y)_{1-x}$ (Se or S)$_x$ was examined as functions of internal strain (inferred from IR spectra) and applied pressure. The session on chalcogenides led off with an excellent tutorial on the photodarkening process. Defects thought to involve under and over coordinated chalcogen atoms are presumably the precursors for optically induced, paramagnetic configurations which absorb light. Other papers in the session discussed photoconductivity studies of As_xSe_{1-x} glasses in terms of these defect levels, as well as a means of doping chalcogenide glass films with high enough concentrations of Al, Cd, and Cu ions to dominate conductivity effects.

The session on theory and modeling commenced with a stimulating paper on the elastic properties of glasses. Building on a model dating from the 1864 work of Maxwell, a force constant model was developed which indicated (among other things) that networks with mean coordination numbers >2.4 are stable. The next two papers dealt with computer modeling of network glasses by molecular dynamics methods. In the first, it was shown that defects taking the form of atoms with coordination numbers differing from the average are intimately involved in diffusion and viscous flow. In the second, vacuum fracture of silica glasses was modeled, indicating nonbridging oxygens and edge-sharing tetrahedra as surface defects. The final paper of this session treated the topological origin of the surface singularities in glasses.

Only two papers were presented on the topic of short-range order. The one described the use of Mossbäuer spectroscopy as a local probe of short and medium range order in network glasses. It was pointed out that, whereas Raman spectroscopy gives information concerning the bond structure of glasses, Mossbäuer probes the site. Experimental results for chalcogenides as As and Ge illuminated both similarities and important differences between Mossbäuer site signatures of crystals and glasses. The other paper of the session treated the mixed alkali effect in alkali aluminogermanate glasses and its experimental dependence on the presence or absence of nonbridging oxygens.

The session on dopants and impurities opened with an extremely comprehensive overview of fluoride glasses for optical applications. In this paper, as in several others which dealt with the more traditional oxide glasses, heavy emphasis was placed on the optical absorption and emission spectra of doped-in transition metal ions as they relate to the potential operation of all-glass lasers. Two papers discussed the local atomic environments of the dissolved transition group ions as revealed by optical and x-ray spectroscopies. Also reported was the use of fast charge transient photoconductivity to probe the electronic structure of arsenic selenide glasses with and without doping with Ni or In.

The unifying theme of the session on fibers and films was the pervasive use of ESR to characterize defect centers. The opening talk was a wide-ranging review of the defect centers and their optical absorption spectra in glass optical fiber wave guides. Summarized were the ESR spectra and ESR optical correlations which have been obtained for the radiation induced defect centers in pure silica, silica doped with Ge, P, or B, and heavy metal fluoride glasses. Other talks reported UV radiation induced defects in Ge-doped silica fibers, gamma-ray-induced defects in P-doped silica fibers, and defects occurring in As-deposited thin dielectric films.

The overview talk of the session on gel-derived glasses contrasted the types of defects expected in glasses produced by that low-temperature route with those defects frozen in during the quenching of melt glasses. Raman data for porous silica gels were presented which strongly indicated surface ring closure as a dehydroxylization reaction. Another paper reported Raman evidence for systematic changes in both surface and internal ring statistics as a function of vacuum heating of a silica aerogel. Two of the papers in the session made mention of the observation by ESR of large concentrations of superoxide radicals in sol-gel silicas following exposure to ionizing irradiations.

The highlight of the final session of the symposium was a well-illustrated lecture showing that 13 of the 15 causes of color in nature apply to glasses. Other papers in the session described new experimental results relating to the thermal conductivity of some flouride glasses and the influence of quenched defects on the thermal expansion and glass transition in diopside glass. Another intriguing contribution dealt with the relationship of Raman spectroscopic measurements to PO_4 chain length (as determined by liquid chromatography) in glasses of the lead iron phosphate system.

Principal Symposium Support: Defense Advanced Research Projects Agency, Hoya Optics, Inc., Lawrence Livermore National Laboratory, Office of Naval Research, Rome Air Development Center,

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Sandia National Laboratories, Schott Glass Technologies, Inc., Xerox Corporation.

Supplemental Symposium Support: American Ceramic Society

Proceedings: Volume 61 of the Materials Research Society Symposia Proceedings series.

Materials Problem Solving with the Transmission Electron Microscope (Symposium Q)

Symposium Organizers: L. W. Hobbs, Massachusetts Institute of Technology; K. H. Westmacott, Lawrence Berkeley Laboratory; D. B. Williams, Lehigh University

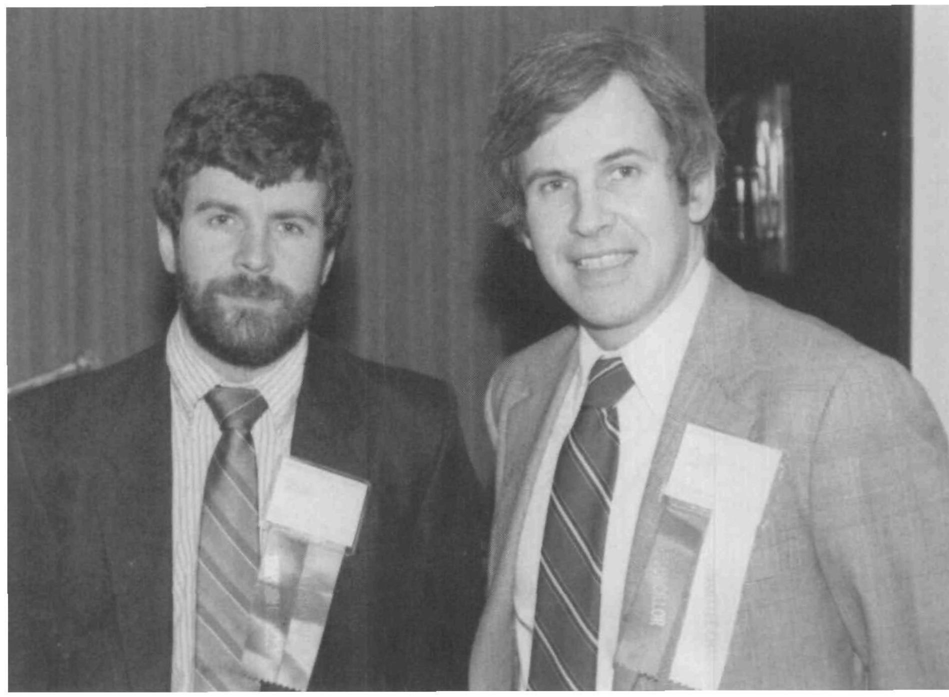
At the symposium on Materials Problem Solving with the Transmission Electron Microscope, 58 papers were presented in six sessions covering a range of materials problems and a variety of microscopy techniques. Seventeen invited papers presented general overviews of the state of our understanding of different materials on a microscopic level, often emphasizing specific advantages gained by using the high spatial resolution available with modern transmission electron microscopes.

The first two sessions focused on electronic materials. A number of papers showed impressive high-resolution micrographs of defects and interfaces, demonstrating that high-resolution microscopy has become a widely applicable and useful characterization method. It was pointed out that the attainable resolution is now often limited not by the microscope itself but by the excessive thickness or contamination of the specimen. Specimen preparation techniques were discussed in a number of papers with a particularly interesting contribution on the use of iodine to replace argon in ion-milling of II-VI compound semiconductors.

The session on analytical electron microscopy had interesting contributions on EDS, EELS, ALCHEMI, CBED and critical voltage with applications ranging from chemical analysis of carbides and nitrides to phase identification in Al-Li alloys.

The application of all techniques of TEM to the analysis of precipitates and phases, transformations and amorphization was the theme of the two following sessions. Examples were given of the use of EDS in work with complex phase diagrams and in segregation and precipitate identification, application of crystal symmetries to morphological analyses, TEM characterization of amorphized and quasicrystalline alloys. The typical breadth of these sessions was perhaps most apparent in a study of the atomic mechanisms of precipitate growth in Al-Ag alloys.

The final session of this symposium concentrated on catalysts and ceramics with contributions on the morphology, composition and bond character of catalyst particles and surface films.



Symposium Q Organizers (left to right): D.B. Williams and L.W. Hobbs.

Symposium Support: JEOL USA Inc., NSA Hitachi, and Philips Electronics Instruments.

Proceedings: Volume 62 of Materials Research Society Symposia Proceedings series.

Computer-based Microscopic Descriptions of the Structure and Properties of Materials (Symposium R)

Symposium Organizers: J. Broughton, State University of New York; W. Krakow, IBM T. J. Watson Research Center; S. T. Pantelides, IBM T. J. Watson Research Center

Everyone will agree, Symposium R was a great success. It was the first symposium of its kind at an MRS Meeting. Judging by the reaction of the participants, it will not be the last. By deliberately mixing the content of the sessions, band structure theorists, Hartre-Fock cluster chemists, computer architects, spectroscopy modelers, and simulationists were brought together in a natural and fruitful way. The breadth of the conference was tremendous; below we try to do some justice to the many areas covered.

In the cross-disciplinary spirit of the conference, three speakers discussed calculations in which electronic properties are evaluated at the same time as walking through phase space by statistical mechanical methods. Carr described a method to evaluate total energies and forces at each time step using density functional theory by employing a formalism in which Newtonian mechanics is used to solve for the electronic and atomic degrees of freedom in the system. Landman coupled pseudo potential and second-order perturbation theory to obtain density-dependent potentials for use in the simulation of nearly free electron metallic glasses. Broughton used a potential parameterized to fit the S(q) for different phases of silicon to generate liquid configurations of silicon atoms which were then employed in a carefully parameterized tightbinding calculation to obtain electronic properties of the liquid state.

Rather than discuss results of direct large-scale calculations, two speakers described alternative ways of obtaining system properties starting with either pseudopotentials or band structures. Hafner, using norm-conserving pseudopotentials and a range of reference states, described a variety of perturbative and variational methods for obtaining liquid and alloy structure factors, melting curves for simple metals, and alloy phase diagrams. P. B. Allen, starting with calculated band structures and experimental phonon energies, showed how it is possible to obtain reliable transport properties and superconducting transition temperatures of transition metals.

The band structure theorists discussed methods to explain surface reconstruction (Freeman, Pandey), to obtain the electronic properties of surface overlayers (Freeman), to examine semiconductor junctions (Van de Walle), to determine the energy of point

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Symposium R Organizers (left to right): W. Krakow, J. Broughton, and S.T. Pantelides.

defects in silicon (Pantelides), to look for magnetic phases in transition metals as a function of pressure (Marcus) and to predict phase transition pressures in transition metals (Anderson) and sp bonded systems (Cohen) using total energy calculations. Cohen described the first fully *ab-initio* calculation of a superconducting transition temperature (in high-pressure hexagonal silicon) by direct evaluation of the electron-phonon coupling.

Several speakers discussed methods for obtaining (and results obtained by using) non-pairwise potentials. Foiles and Jacobsen discussed the embedded atom technique for transition metals while Weber, Wetzel, Biswas, and Dodson described many-body silicon potentials as applied to surfaces, extended defects, and bulk phases. Tersoff was in the audience distributing his new silicon potential. Raghavarchari and Schluter (in audience) described *ab-initio* Hartre-Fock and density functional calculations on small clusters of silicon atoms against which to parameterize future silicon potentials.

Hartre-Fock cluster calculations were discussed by five speakers (see also above). Goddard described calculations to elucidate chemical reaction pathways on the surfaces of molybdates; Malvido discussed vibronic couplings in the neutral vacancy of silicon; Hao described cluster calculations aimed at determining surface structures of silicon; and Vail described a user-friendly package for obtaining vacancy energies and states in ionic solids.

Four speakers addressed the issue of computer-based analysis of spectroscopic and microscopic studies of grain boundaries, inclusions, and interfaces. Mills described a multiple scattering theory of the excitation cross-secton for surface electron energy loss spectroscopy. Shapiro discussed a computer simulation of sputtering from two component liquid metal targets, and Krakow described image interpretation of electron microscope images by computer modeling of the electron scattering processes in the sample. Last, Varadan discussed the T-matrix approach for calculating frequency dependent dielectric properties in composite materials.

Turning now to defective solids, computer simulations of glassy materials were described by Angell and by Lancon. Vitek described the highly degenerate structure of grain boundaries. Cormack presented a method for obtaining diffusional activation energies in ionic systems using shell models embedded in a continuum. The dynamics of polymers in micelles were described by Haile, and Turner discussed the response of polymer systems to external force. Simulations to describe grain growth and grain size distributions were presented by Anderson and by Frost.The simulation of fragmentation patterns was discussed by Brostow.

Path-integral methods were presented by Dolla and by Landman. The former described Monte Carlo techniques to determine equilibrium and dynamical properties in a range of condensed phase quantum-mechanical systems; and the latter described a path-integral molecular dynamics simulation of electron localization in NaCl clusters.

There were many papers aimed at elucidating and understanding the structure of interfaces. D. C. Allen discussed a total energy tight binding method for examining surface phonon modes and surface structures in silicon. Landman described molecular dynamics simulations of silicon crystal melt interfaces. Rosato presented molecular dynamics results for high-temperature Lennar-Jones crystal-vapor surfaces aimed at determining surface diffusion coefficients. Jackson described molecular dynamics and Monte Carlo simulations of crystal growth and surface roughening.

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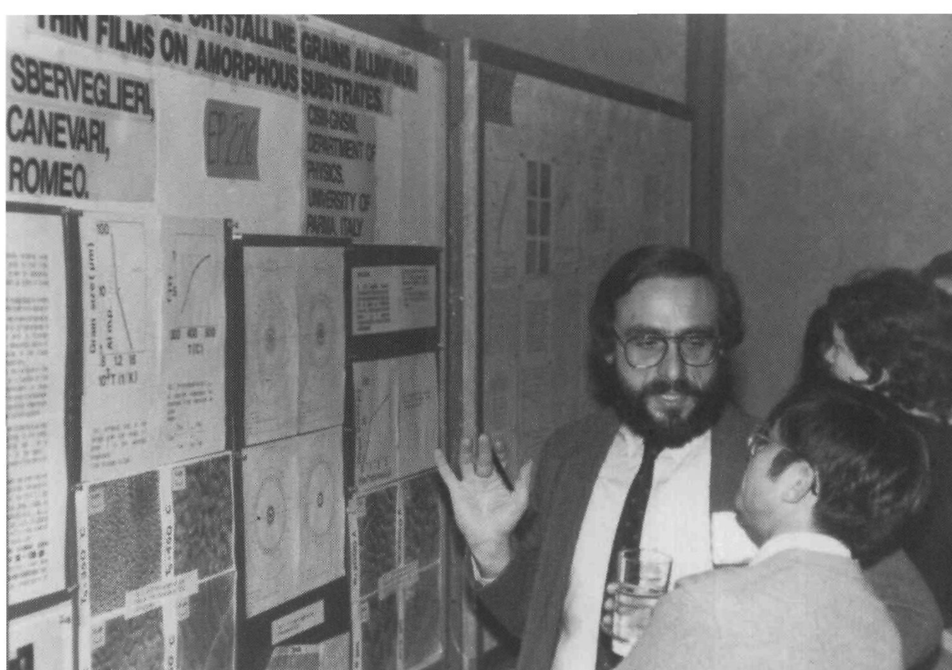

Poster Session.

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Laird described molecular dynamics results for a model bcc-melt interface and compared them with the predictions of an order-parameter theory for the same system.

Last, four speakers described computer architectures for dedicated simulation. Bakker presented an overview of the many existing machines used for Monte Carlo-spin and molecular dynamics-continuous-coordinate simulations with special emphasis on his many-stage pipe-lined molecular dynamics machine. Ogielski described his Monte Carlo-spin processor used in examining the behavior of spin glasses. Carleton and Auerbach described true parallel processor architectures for molecular dynamics simulations.

By way of overview, Eberhardt presented the findings of a DOE report on the hierarchical nature of the design of new materials emphasizing the need for a firm foundation of first principles calculations. He cited the example of modeling of grain boundary adhesion in Ni_3Al. Last, Hoover gave a five-strategy approach to extending simulation at the atomic level to determining the macroscopic properties of real materials; ranging from mesoscopic simulations to techniques of nonequilibrium molecular dynamics.

One was struck at this conference by a sense of excitement: there really are many properties that can be calculated by first principles methods to a high degree of accuracy (e.g., the phase diagrams of high-pressure crystals, the reaction pathways of surface catalysis, the transport properties of transition metals); new ways of thinking about exposing the underlying trends in materials behavior are being developed (e.g., theories of crystal-melt interfaces, perturbative approaches to the structure of sp-bonded alloys, crystals and liquids); and people are starting to think of ways to combine *ab-initio* methods with statistical mechanical simulation. By the time the next symposium of this type is held, we can anticipate many new and exciting developments in the computational physics of materials.

Symposium Support: National Science Foundation, Department of Energy-Oak Ridge Army Research Office, IBM Corporation, CSPI Inc., Air Force Office of Scientific Research, and NASA Lewis Research Center.

Proceedings: Volume 63 of Materials Research Society Symposia Proceedings series.

Cement-Based Composites: Strain Rate Effects on Fracture (Symposium S)

Symposium Organizers: S. Mindess, University of British Columbia; S. P. Shah, Northwestern University

This symposium reflected the increasing interest in the effects of strain rate, and in particular the high strain rates associated with impact or impulsive loading, on the fracture properties of concrete. As is inevitable in a symposium such as this one, a wide variety of topics was covered, ranging from crack growth studies in cement paste to the development of an impact model of concrete. Both experimental and theoretical papers were presented. However, a common thread ran through most of the papers: the strain rate effects were interpreted, either explicitly or implicitly, in terms of fracture mechanics.

Symposium S Organizers (left to right): S. Mindess and S.P. Shah.

The theme of the symposium was set by the four invited papers. F. H. Wittmann (Ecole Polytechnique Federale de Lausanne) suggested that while LEFM can be used to characterize crack propogation in relatively brittle materials, such as hardened cement paste and autoclaved aerated concrete, it does not work for concrete. For concrete, a nonlinear fracture criterion, such as Hillerborg's fictitious crack model, must be used. He also suggested that rate theory provides a basis for interpreting the strain rate dependence of the fracture of concrete. In a complementary paper, H. W. Reinhardt (Delft University of Technology) dealt primarily with strain rate effects on the tensile strength of concrete. He argued that, at relatively low strain rates, rate theory could be used to relate strain rate and tensile strength. At very high strain rates ($>10^3$/s), the strain rate effect is due entirely to dynamic effects (inertia). At intermediate strain rates, both rate processes and dynamic effects must be considered. L. E. Malvern (University of Florida) described extensive experimental studies, using a split-Hopkinson's Pressure Bar, on the dynamic compressive strength of cementitious materials. Tests were carried out at strain rates of up to 800/s on mortar, and 120/s on concrete. He showed that, at the higher strain rates, at least some of the apparent strain-rate effect is really due to lateral inertial confinement of the concrete. Finally, S. P. Shah (Northwestern University) described the model that he and his co-workers have developed to describe the fracture of concrete, in which slow (pre-peak) crack growth is considered in calculating the fracture parameters. He showed that the log V vs. Log K_I relationship is nonlinear, with the slope (m) of the log V vs. Log K_I plot increasing sharply at high rates of loading. However, he suggested that, because of the decrease in pre-peak crack growth at high strain rates, it might be valid to use LEFM at very high rates of loading.

The contributed papers fell into different categories. Several papers dealt with the use of continuum damage mechanics to describe the dynamic fracture of concrete. Using this approach, a cube-root relationship between strain rate and strength of a very high strain rates can be predicted; this is consistent with some of the experimental data obtained at these strain rates. Time-dependent void growth was also used to model damage accumulation and the consequent strength reduction.

The majority of papers, however, dealt with experimental studies. On the more fundamental side, there were several dis-

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cussions of the determination of fracture toughness parameters for ordinary and MDF cements, and for concrete. On every interesting contribution by Darwin and Attiogbe (University of Kansas) dealt with a study of submicroscopic cracking in cement paste as a function of loading rate. They showed that, for loading to a fixed strain rate, slow loading results in less cracking than rapid loading; however, at the same stress/strength ratio, rapid loading results in fewer cracks.

A number of papers dealt with impact or impulsive loading of plain concrete, fiber-reinforced concrete, and conventionally reinforced concrete. Takeda (Kumamoto Institute of Technology, Japan) showed that crack velocities were related to the strain rate; he was able to achieve measured crack velocities of up to about 1000 m/s. Other researchers were only able to achieve much lower crack velocities, in the range of 100-200 m/s. However, these values are all well below the "theoretical" terminal crack velocity in concrete, of about 1600 m/s. Kobayashi, Hawkins, and Du (University of Washington), using both experimental and numerical studies, were able to develop an impact model for concrete, which could be used to provide reasonable prediction of the behavior of plain concrete beams under impact loading. They too suggested that the reported strain rate sensitivity of concrete might be attributed in part to the dynamic state of stress, and might therefore not totally be an inherent material property.

The symposium concluded with a discussion by J. Hager (Air Force Office of Scientific Research) on the U. S. Air Force research and funding initiative on cementitious materials. He described the applications of concrete in which the Air Force had particular interest, such as runways and blast and impact resistant structures. He concluded on a hopeful note, with the thought that a materials science approach might be used systematically to improve concrete properties, as it had with ceramic materials.

From the papers and discussions, it became clear that much remains to be learned about the properties of concrete at very high strain rates greater than about 100/s. This is particularly the case for reinforced concrete elements and structures. Most of the test results presented were obtained from small, laboratory-scale specimens; few data are available for large structural elements. However, if adequate design codes for concrete structures subjected to high strain rate loading are to be developed, both more experimental work and more sophisticated numerical methods must be carried out.

Symposium Support: Air Force Office of Scientific Research, Army Research Office, W. R. Grace & Co., Portland Cement Association, Elkem Chemicals, Inc., and Martin Marietta Laboratories.

Proceedings: Volume 64 of Materials Research Society Symposia Proceedings series.

Equipment Exhibit.

Fly Ash and Coal Conversion By-Products: Characterization, Utilization and Disposal II (Symposium T)

Symposium Organizers: G. J. McCarthy, North Dakota State University; D. M. Roy, Pennsylvania State University

This symposium, the fourth such MRS symposium held on this topic, was concerned with the scientific aspects of characterization and utilization of the by-products generated when coal is burned or gasified. Forty-two papers were presented in a 2½ day symposium which opened with a consideration of the interface between research and technology. Numerous aspects of fly ash beneficiation and mineral recovery, production methods and energy conservation implications, and the effect of types of production and quality on the potential utilization in the United States, Western Europe, and Australia were discussed.

A critical paper on characterization of the inorganic constituents in coal presented by R. B. Finkelman (Exxon) set the stage for determining the characteristics of the fixed-bed by-products. Characterization of the inorganic constituents was found to be complicated by: (1) the small size of the minerals (mean grain size is less than 5μm); (2) intimate association of the organic and inorganic phases; (3) complex and variable mineral assemblages; (4) rare but environmentally important accessory mineral phases; and (5) modifications created by handling and analysis. Papers by G. J. McCarthy (North Dakota State University) and R. J. Stevensen (University of North Dakota), R. T. Hemmings and E. E. Berry (Ontario Research Foundation, Canada), H. Roper (University of Sydney, Australia), T. Demirel (Iowa State University), S. Diamond (Purdue University) and R. W. Linton (North Carolina State University) presented detailed characterization of fixed bed gasification ash and fly ash from vastly different regions, types of coal, and firing conditions. SEM, XRD, ICAP, XANES, EXAFS, SIMS, BET, SIM, BET, particle size analysis, and bulk chemical analysis are among the methods used.

Other papers dealt with the effects of particle characteristics on reactivity in the alkaline medium of hydrating Portland cement concrete, a major product for utilization of such ashes. Available or soluble alkalis in the fly ash were found to be important in governing the fly ash reactivity (T. Demirel, Iowa State University).

Numerous studies were reported on the characteristics and properties of cement paste or concrete incorporating amounts of fly ash. The hydrating fly ash-cement paste matrix was shown to be effective in adsorbing or fixing chloride anions, diminishing their mobility. Pore fluid expression techniques and analyses were used by D. M. Roy and co-workers in the latter study,

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and by F. P. Glasser et al. to investigate the changing pore fluid composition in cement paste-fly ash systems during early hydration. A. Kumar and D. M. Roy used diffusion techniques combined with pore structure analysis to determine the ionic transport and related properties of such cementitious materials. Blends containing Portland cement with low-calcium fly ash showed significant retardation of both Cs^+ and CL^- ionic diffusion when compared with normal Portland cement.

Other papers related the mineralogy, morphology and chemical composition of fly ashes to their reactivity with alkaline cement mixtures. Microstructural changes taking place in fly ash-cement pastes and concrete with time were investigated. Thermogravimetric, x-ray diffraction, scanning electron microscope, and mercury porosimetry methods have been used to determine phase changes and microstructural changes occurring as a result of chemical reactions, such as through carbonation.

The development of fly-ash reference standards through an NBS-PCA cooperative effort was described. Further important developments reported were the formation of fly-ash data centers at Iowa State University, University of North Dakota and North Dakota State University; and University of Calgary.

Attempts to use basic characteristics of fly ash to model the development of properties of concrete containing fly ash were described from studies at Dunstan, Inc. (Lakewood, CO) and at Pennsylvania State University, which used somewhat complementary approaches and methodologies.

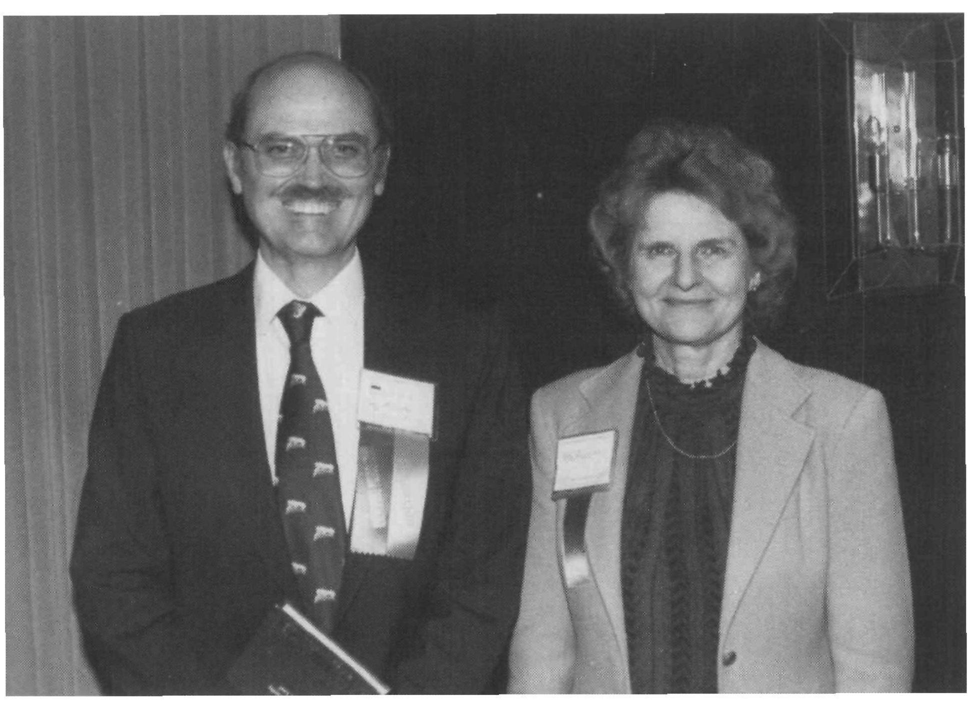
The results of characterization studies of fly ash related to effective disposal were summarized by Murarka (EPRI). A scientific basis for disposal comes from equilibrium and kinetic data on precipitation/dissolution and adsorption/desorption mechanisms that operate in wastes and soils, and subsurface transport processes in the water medium. The leaching behavior of fixed-bed gasification ash was investigated by the North Dakota researchers. In order to suggest which phases in the ash were controlling the solubility of the major elements in the ash, a geochemical modeling computer code was used. Leaching behavior of the trace elements were discussed in terms of RCRA, drinking water and irrigation water standards. Penn State researchers described the leaching characteristics of fly ash and fly ash-cement mixtures, exploring the potential for utilization as a bedding base material. They also reported characteristics and properties of a type of cementitious material prepared with large proportions of fly ash, developed (with Savannah River Laboratory) to solidify saline low-level nuclear waste solutions. Thermal properties (conductivity, heat capacity, adiabatic heat of hydration) and x-ray diffraction and microstructural characterization, along with leaching properties and ionic diffusivity were used to evaluate the cementitious waste forms.

This symposium emphasized the progress made during the past year in integrating knowledge gained on this complex type of material.

Principal Symposium Support: Electric Power Research Institute, National Science Foundation, American Fly Ash and Army Research Office.

Co-sponsors: North Dakota Mining and Mineral Resources Research Institute and Western Fly Ash Research, and Development and Data Center.

Proceedings: Volume 65 of Materials Research Society Symposia Proceedings series.



Symposium T Organizers (left to right): G.J. McCarthy and D.M. Roy.

Frontiers of Materials Research (Symposium X)

Symposium Organizer: Rustum Roy, Pennsylvania State University

When the founders of the Society were putting together the first few annual meetings of the Materials Research Society the concept of MRS being the place where the membership—and the outside world—could always get a view of the "frontiers" of materials research was formed. "Frontiers of Materials Research" became and remains the title used annually by Symposium X. This unique symposium provides reviews of the latest developments for the non-specialist. Some of the reviews covered during this symposium at the 1985 Fall Meeting were: clays and zeolites, amorphous materials, surfaces and thin films, ion implantation in semiconductors, semiconducting and metallic polymers, and materials for lasers.

On Wednesday, Symposium X departed from its usual practice and presented not a review but a first-time-ever announcement of a major research advancement: The Lanxide Process. The two papers presented by Marc Newkirk, the developer of the process, and his colleagues at the Lanxide Corporation, Wilmington, Delaware, provided the first public disclosure of the science underlying the process. The papers, titled "Formation of the Lanxide Ceramic Composite Materials" and "Properties and Microstructures of Selected Lanxide Composite Materials," explained that the process uses a $L+V \rightarrow S$ mechanism to make a free-standing polycrystalline, dense ceramic object. While the papers noted that the same process has been applied to a wide variety of materials, details were provided basically on the system $Al + O_2 \rightarrow Al_2O_3$.

Molten aluminum appropriately doped contained in a ceramic container may be oxidized in air at 1000-1300° C to yield a ceramic body. There appears to be no obvious limit to the size of the object made, and the process is simple and relatively rapid.

The report included a wealth of detail on the unique microstructure of the materials produced, consisting of oriented α-Al_2O_3 grains showing very low angle grain boundaries between them, and incorporating varying amounts of aluminum-metal. This

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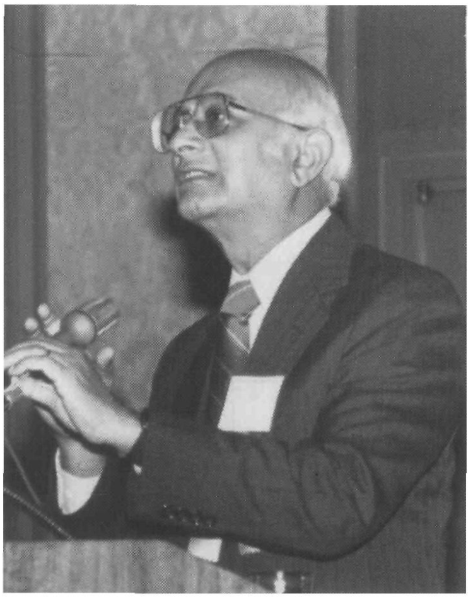

Symposium X Organizer: R. Roy.

metal-ceramic composite arrangement confers various desirable properties such as increased work to fracture on this class of materials. The author also presented hypotheses on why the process works. The use of coupled dopants, e.g., magnesium silicon, appear to be necessary, and the transport of the aluminum through the forming Al_2O_3 ceramic is attributed to the differences in surface tension between the Al_2O_3 and the metal in the absence and presence of air.

Editor's Note: The first issue of Journal of Materials Research *includes a full discussion of The Lanxide Process. See "Journal of Materials Research Premier Issue Nears Completion" in this issue of the* BULLETIN.

Frontiers in Materials Education (Symposium Y)

Symposium Organizers: G. L. Liedl, Purdue University; L. W. Hobbs, Massachusetts Institute of Technology

The symposium on Frontiers in Materials Education reviewed the status and challenges across the spectrum in materials education. The symposium included 10 invited papers and 12 contributed papers. Throughout this well-attended, two-day symposium, it was clear that education in materials science and engineering is undergoing dynamic changes reminiscent of the 1950s and 1960s. The breadth of the field with the multitude of factors that impact the educational system was evident. Also, it was apparent that the field is still in an expanding multidisciplinary mode and has not coalesced into a cohesive discipline. A spectrum of ideas, concepts, changes, programs, and problems were presented.

The first session focused on philosophy and the future. One of the major questions that was present throughout this session was the integrated versus the specialized materials class approach to education in the field. A factor coupled with this question was the historical evolution of the field along with the demands and pressures from industry and other disciplines. Problems relative to an integration of all materials classes were presented. Polymers were noted as a specific problem with major faults in available educational materials. M. Bernstein discussed the Metals/Materials Dichotomy and the evolutionary changes that have occurred in response to a perceived changing environment. Also, M. Flemings introduced an approach to an integrated education in MSE. He addressed directly the question of subjects that span the field for use in such an approach as well as the need and opportunity for new teaching methods and materials. Interdepartmental approaches were presented by H. Marcus, who discussed the relative advantages and disadvantages of such an approach.

The second session focused on interactions of materials education with other segments of the field. The university-industry interactions that have long-range significance to the traditional mission, policy, and infrastructure of the university were presented by J. J. Harwood. Other needs and programs for interactions with industry and national laboratories were addressed by P. Chaudhari and S. Hecker. Also, some innovative programs were presented for microelectronics by M. Russell, for materials in sports by G. Michal, national laboratory programs by J. Rusin, and nondestructive evaluation by Robert Green.

In the third session special problems and new directions for polymers and ceramics were presented by E. L. Thomas and D. Readey. Also, an approach for recruiting of students was presented by S. Stafford, and a computer usage approach was presented by D. Turner.

The final session featured a provoking discussion by R. Roy on cross-disciplinary features of materials education for materials research. Materials education in other disciplines was also presented with a unique approach by The Open University in the UK for electronic materials and devices.

The symposium ended with a general discussion that focused upon the major challenges facing the materials education area. An item of specific interest and discussion was the initiation of a major study, Materials Science and Engineering Study, by the National Research Council. The potential impact of this study was considered to be major and the results of this symposium would serve as one input into the study.

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Symposium Y Organizers (left to right): G.L. Liedl and L.W. Hobbs.

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