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RESEARCH NOTES

Volume 1 Number 1

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Quantitative identification of siliceous species in zeolite magma

Growth of large diameter, low dislocation density single GaAs crystals

Reversal of the substrate charge specificity of an enzyme

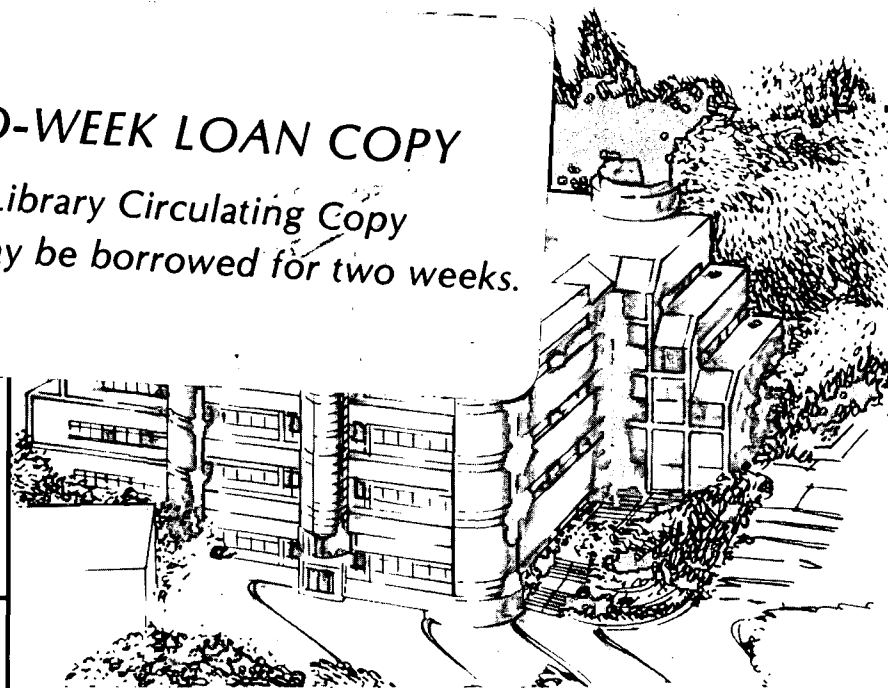
Superior properties of lithium-aluminum alloys at cryogenic temperatures

Splitting and delamination of vapour deposited chromium films

Intel and Catalytica send Industrial Fellows to Interface and Catalysis Programs

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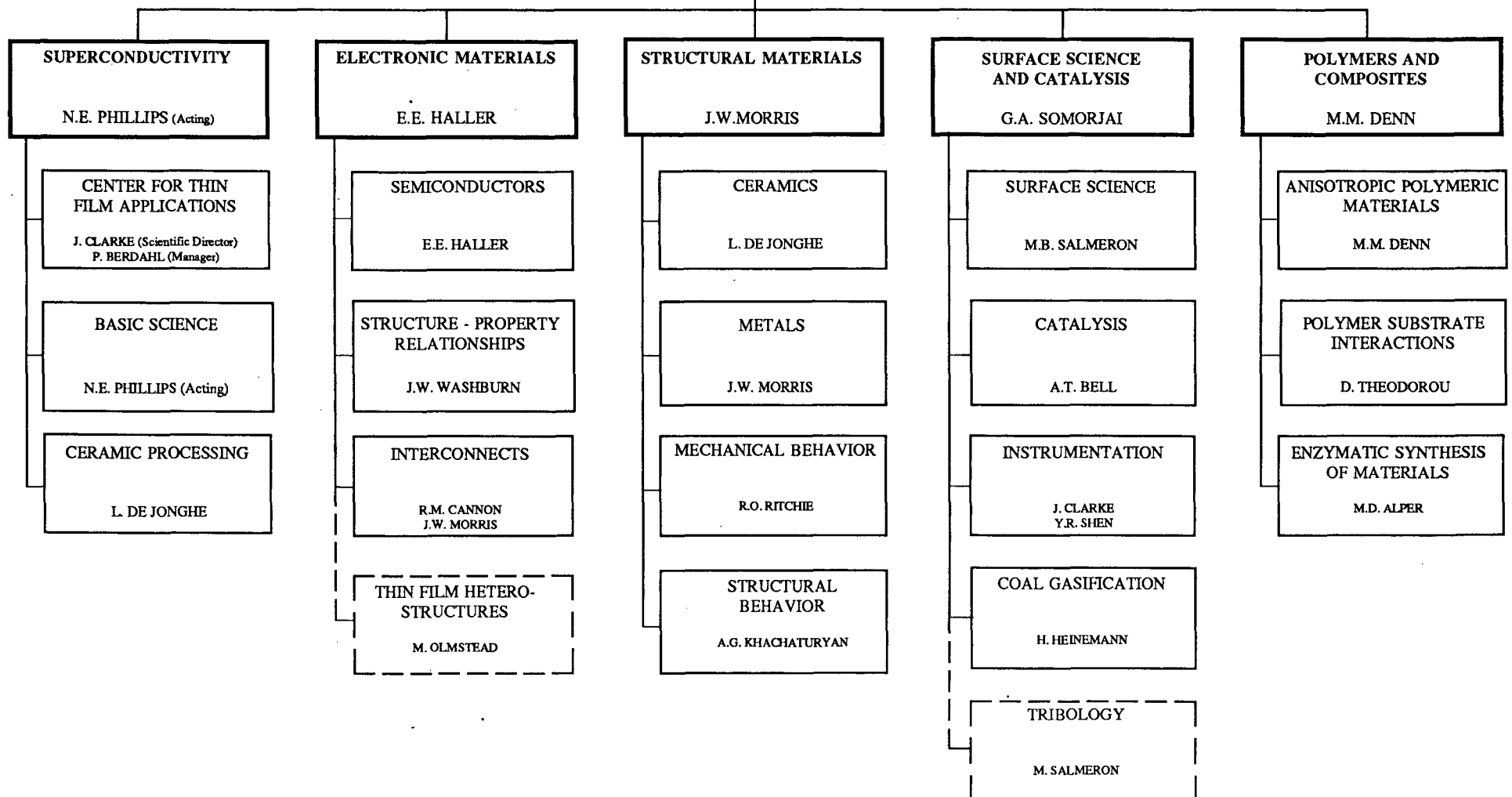
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The Center for Advanced Materials was established in 1983 and receives major funding from the U.S. Department of Energy, Office of Basic Energy Science. Its mission is to perform basic research in areas of materials science of importance to U.S. industry. We welcome communication from any industrial research groups interested in collaborations or other interactions with the CAM programs.

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INSTRUMENTATION FOR SURFACE SCIENCE

John Clarke, Program Leader

REMARKABLE ASYMMETRY OBSERVED IN GRAPHITE

A scanning tunneling microscope (STM) built by the Center for Advanced Materials' Instruments and Sensors Program at LBL has the ability to resolve single atoms on the surface of electrically conducting samples. Images of graphite have been obtained in the "current-imaging" mode, where variations in tunneling current give information about the topology and electronic structure of the surface. Carbon atoms in the honeycomb array are clearly visible but surprisingly, they exhibit an enormous asymmetry, with alternate atoms appearing grey (α) or white (β). The two types of atomic sites do in fact differ in that the α carbons have neighboring atoms in the atomic layer below while the β carbons do not. *Ab initio* calculations, performed by the program's theorists have demonstrated that the asymmetry is due to details in the electronic band structure of the graphite near the Fermi energy E_F . The particular symmetries of the electronic states on the α and β atoms near E_F were shown to cause an asymmetry in the corresponding charge densities in the specific narrow energy region sampled by the STM. Thus, the features observed experimentally are well explained by the theory. These results demonstrate the usefulness of the STM for investigating the fine details of electronic structure and the forces that influence them. The risks inherent in interpreting STM images simply in terms of atomic charge densities are also very well illustrated.

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POLYMERS

Morton M. Denn, Program Leader

SHAPE, STRESS DISTRIBUTION AND INSTABILITY PREDICTION IN POLYMER PROCESSING

Computational research in the Center for Advanced Materials' Polymers Program has led to the development of an accurate and efficient approach to the prediction of shapes, stress distributions, and instabilities under conditions when there is a polymer/gas interface during processing of the polymer. Using this approach and guided by calculations on the CRAY X-MP supercomputer and extrusion experiments, CAM researchers have identified a physical basis for the general inability of researchers worldwide to be able to predict polymer flow and structure development in complex mold shapes. This work has demonstrated the need for a better understanding of the interactions between a polymer melt and a metal surface before control of the process and therefore of the properties of the polymer product can be achieved.

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SURFACE SCIENCE AND CATALYSIS**Gabor Somorjai, Program Leader****QUANTITATIVE IDENTIFICATION OF
SILICEOUS SPECIES IN ZEOLITE MAGMA**

In work with supplemental support from W. R. Grace Company and the Harshaw/Filtrol Partnership the Center for Advanced Materials Catalysis and Surface Science Program at LBL has employed ^{29}Si NMR spectroscopy successfully to identify and measure quantitatively the siliceous species present in the magma from which A and Y zeolites are grown. The spectra obtained with a high-resolution 500 MHz spectrometer indicate the presence of monomeric silicate anions and oligomeric species containing 2 to 12 Si atoms linked via siloxane bridges. Thus far, 19 distinct structures have been identified, many of which contain 3, 4, and 6 membered rings. The presence of zeolite secondary building units, such as the cubic octamer and double hexamer, have also been established. For a fixed silica concentration the absolute concentration of a given species is a sensitive function of $\text{SiO}_2/\text{Na}_2\text{O}$ ratio. The ability to follow the synthesis of zeolites during the early stages of their synthesis is a major step towards the goal of learning how to control reaction conditions to achieve synthesis of zeolites of predetermined structure and function.

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ELECTRONIC MATERIALS**Eugene Haller, Program Leader****GROWTH OF LARGE DIAMETER, LOW DISLOCATION
DENSITY SINGLE GaAs CRYSTALS**

The Center for Advanced Materials' Electronic Materials Program at LBL has implemented the techniques to grow large diameter (2" and 3") low dislocation density (less than $5 \times 10^3 \text{ cm}^{-2}$) single crystals of gallium arsenide using Electro-Dynamic Gradient Horizontal Bridgman furnaces. The unique design of the furnace together with the computerized control system provide exceptional reproducibility of the growth cycles. Extensive studies of thermal profiles in the growth furnaces and their relationship to the shape of the solid-liquid interface during the growth allowed the optimization of growth conditions for crystals with specific properties. Precise control of arsenic pressure is used for understanding of stoichiometry effects on electrical (resistivity) and structural (dislocation density) properties of the crystals.

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ENZYMATIC SYNTHESIS OF MATERIALS

Mark Alper, Program Leader

REVERSAL OF THE SUBSTRATE CHARGE SPECIFICITY OF AN ENZYME

Scientists in the Enzymatic Synthesis of Materials Program of the Center for Advanced Materials have, for the first time specifically altered an enzyme so that it catalyzes a chemical reaction using a substrate with a charge opposite to that of the substrate it uses in Nature. This represents a significant step towards the demonstration of the feasibility of the program's goal of producing new materials with enhanced properties through the use of enzymes that have been specifically redesigned for that purpose.

Earlier studies of the enzyme aspartate aminotransferase had suggested that positively charged arginine, the enzyme's 292nd amino acid, is in direct contact with the substrate. Thus a substitution of that arginine by the negatively charged amino acid aspartate might be expected to alter the specificity of the enzyme from negatively charged to positively charged substrates. Site-directed mutagenesis was performed, and pure enzyme was obtained with the substitute amino acid. Activity of the new enzyme on the new substrate is 15-fold greater than that of the natural enzyme, and the ratio of activity on the new substrate compared to the old is increased by more than a million-fold.

The arginine in question is only one of the amino acids in the enzyme that contact the substrate; additional amino acid substitutions would likely further increase the enzyme's selectivity towards the new substrate. This ability to alter the substrate specificity of an enzyme is critical to the use of enzymes to produce new polymeric materials.

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STRUCTURAL MATERIALS

J.W. Morris, Jr., Program Leader

SUPERIOR PROPERTIES OF LITHIUM-ALUMINUM ALLOYS AT CRYOGENIC TEMPERATURES

Tests conducted by the Center for Advanced Materials' Structural Materials Program at LBL have shown that the yield strength, ultimate tensile strength, fracture toughness and elongation of the new lithium-aluminum alloy 2090-T81 all improved as temperature decreased to 4° K. Consequently, the strength-toughness combination (the most important design parameter) improves dramatically as temperature decreases. At the lowest temperatures, 2090 is far superior to any aluminum alloy currently used for cryogenic applications. In addition, the results of weldability studies of sheets of the alloy suggest that with appropriate post-weld processing, acceptable welding properties of the material can be achieved. Thus, 2090 can be seriously considered for use in the cryogenic fuel tanks for the space shuttle or the proposed hypersonic and trans-atmospheric vehicles.

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CERAMIC AND METAL INTERFACES**Rowland Cannon, Program Leader****SPLITTING AND DELAMINATION OF
VAPOUR-DEPOSITED CHROMIUM FILMS**

Striking examples of splitting and delamination of low temperature vapour-deposited or electro-deposited Cr films induced by inherent tensile stresses have been observed by the Center for Advanced Materials' Ceramic and Metal Interfaces Program at LBL. Delamination of vapour-deposited chromium is partially in a glass substrate, and primarily 1 to 3 film thicknesses deep within a Si substrate. High interfacial G_c permits local shear stresses to induce the transition to substrate fracture that occurs more readily for Si than for the tougher glass. Atmospheric moisture enhances interfacial or substrate delamination for Cr/glass, but seemingly not for Cr/Si. Low temperature annealing exacerbates decohesion evidently by increasing residual stresses. With some deposition conditions, the ensuing profuse, fine microcracking limits stresses and prevents gross splitting and delamination. Further understanding of these phenomena will lead to methods to improve adhesion of semiconductor interconnects and coatings.

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