Center for Advanced Materials

CAM RESEARCH NOTES

Volume 3 Number 2 *December 1989*

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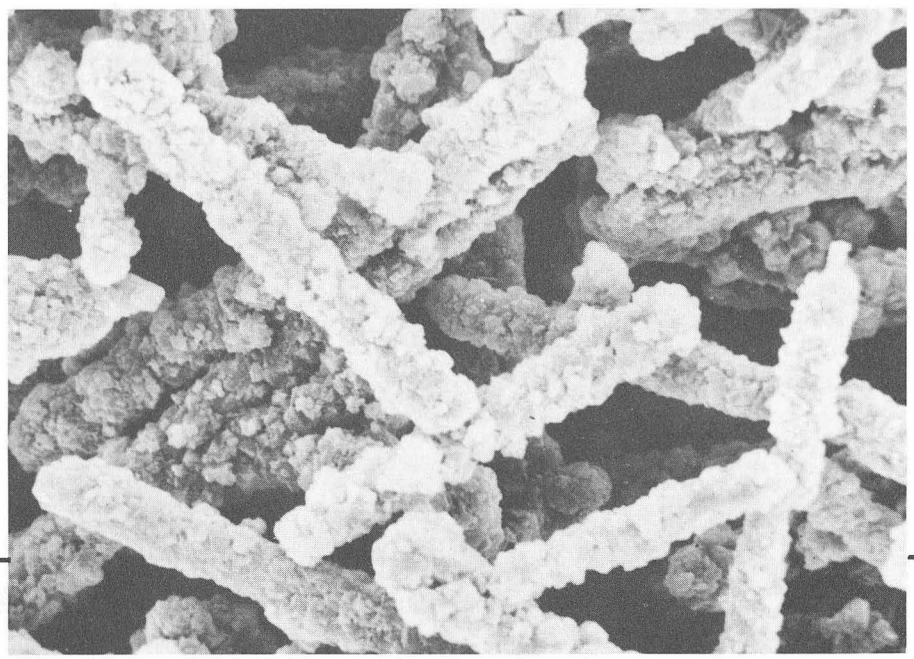

Materials and Chemical Sciences Division
Lawrence Berkeley Laboratory • University of California
ONE CYCLOTRON ROAD, BERKELEY, CA 94720 • (415) 486-4755

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CENTER FOR ADVANCED MATERIALS

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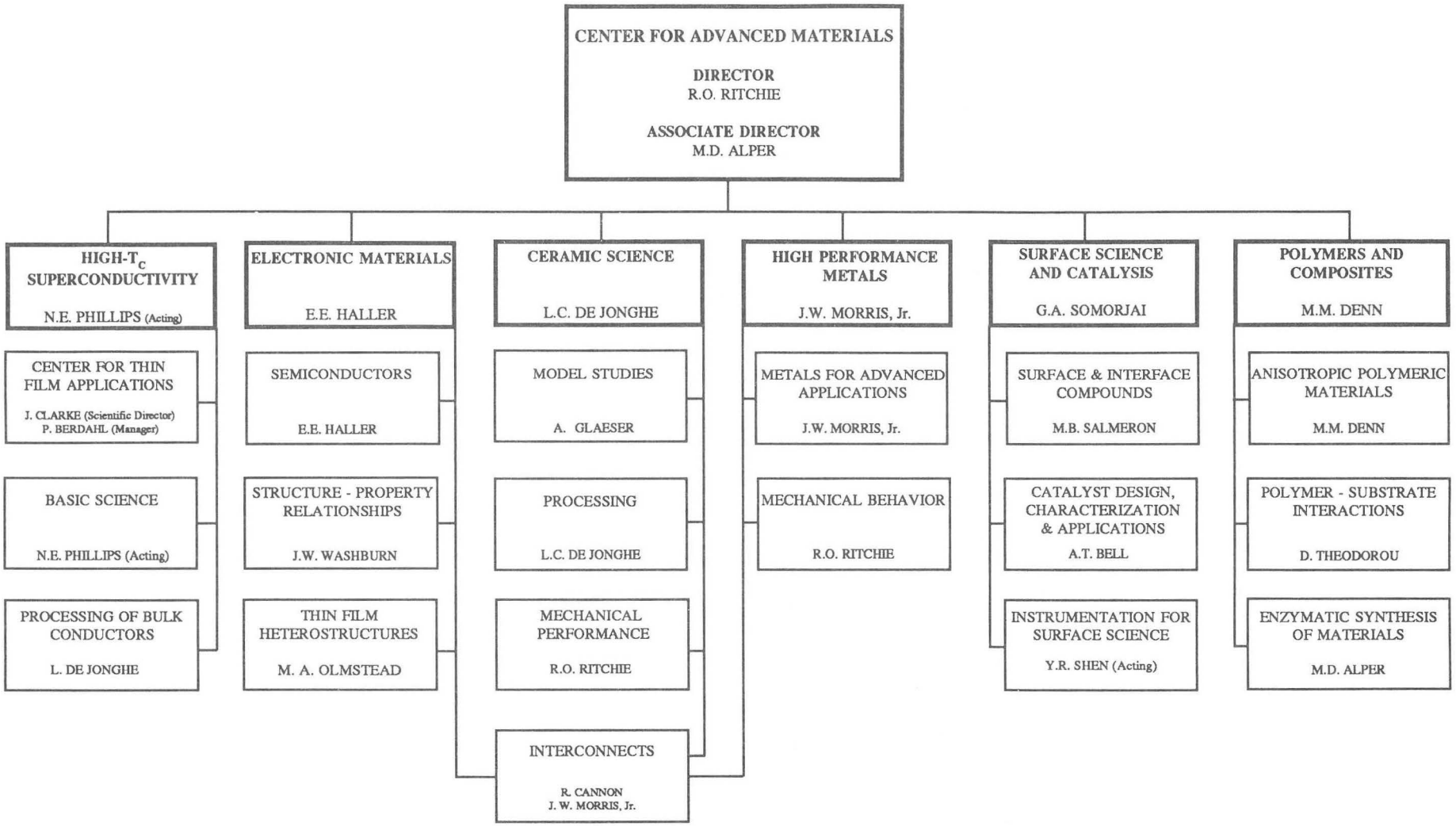
The Center for Advanced Materials was established in 1983 and receives major funding from the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences. Supplemental funding from other agencies is noted as appropriate. The mission of the Center is to perform fundamental research in areas of materials science of importance to U.S. industry. We welcome communication from industrial research groups interested in collaborations or other interactions with the CAM programs.

Cover: Alumina-coated SiC whiskers. These whiskers, originally with diameters ranging from 0.25-3 μm, have been fully coated, preventing direct whisker contacts in the green body. This enhances densification and provides a more uniform distribution of the whiskers in the composite.



Effective 10/11/89

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CAM *RESEARCH NOTE*

INDUSTRY PARTICIPATION

CAM, DOE, CALIFORNIA, STANFORD, AND CONDUCTUS COMBINE EFFORTS TO COMMERCIALIZE 77 K SQUIDS

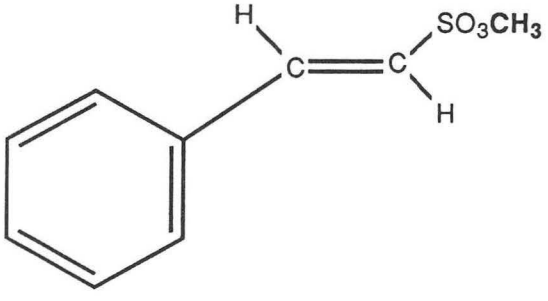
A group in the CAM program on High-T_C Superconductivity, with support from the U.S. Department of Energy, has joined with The State of California, Stanford University and Conductus, Inc., a start-up company in California's Silicon Valley, to apply the results of its fundamental research on Superconducting QUantum Interference Devices (SQUIDs) and the new high-T_C superconducting materials to the production of a device for oilfield exploration and other applications.

The collaboration has several facets. The U.S. Department of Energy, Division of Materials Sciences will continue its long-term support of fundamental research in electronic device development and superconductivity in a program under the direction of CAM project leader John Clarke. In addition, the State of California, as part of its new Competitive Technology Program, will contribute close to one half million dollars over the next 18 months to support the transfer of that technology to Conductus. Conductus will assign one of its senior scientists to work with Prof. Clarke's research group at CAM, with support of the DOE Office of Energy Research Program on Industry-Laboratory Technology Exchange. This program is designed specifically to increase direct interaction between industry and laboratory scientific groups by providing funding for extended visits of industrial scientists to DOE laboratories. Finally, the thin films required for the fabrication of the devices will be produced both by colleagues at nearby Stanford University and at Conductus, Inc.

SQUIDS are the world's most sensitive detectors of changes in magnetic flux. The goal of this project is to demonstrate and develop SQUIDS fabricated from the new high-T_C superconducting materials together with the high-T_C superconducting flux transformer and the electronics necessary to process the SQUID output. The system will be capable of operating at temperatures up to the boiling point of liquid nitrogen, 77 K. Success in the collaboration is likely to have a major impact on certain applications of these SQUIDs because the instruments could, for the first time, be operated unattended in remote areas for many months. Applications such as NMR characterization of the strata surrounding oilfield boreholes, geophysical surveying, active electromagnetic sounding, earthquake prediction, and biomagnetism, in addition to laboratory instrumentation, are forseen. Market development and commercialization will be undertaken by Conductus through private financing.

CAM Industry Participation Office: Mark Alper, (415) 486-6581

a



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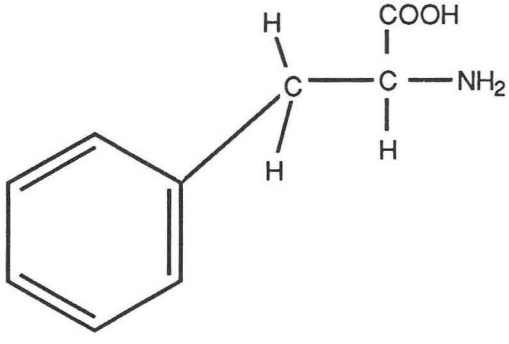

Methyl (β-cinnamoyl) sulfonate (MCS) (a) structural analog of phenylalanine (b), a part of the natural substrate for the enzyme subtilisin. The activated methyl group on MCS (bold) is transfered to the enzyme active site, altering its reactivity and allowing synthesis of polyamides.

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CAM *RESEARCH NOTE*

POLYMERS AND COMPOSITES

BACTERIAL ENZYME ENGINEERED FOR POLYMER SYNTHESIS

Designed modifications of the enzyme subtilisin have been achieved that should significantly improve its ability to synthesize polymers for materials and other applications. The changes involve the substitution of selected amino acids in the enzyme, the chemical alteration of another, and the use of new reaction conditions.

CAM scientists C.H. Wong and J.A. Bibbs, working at the Research Institute of Scripps Clinic, used an enzyme modified by colleagues at the Genex Corporation. Six of the enzyme's 275 amino acids were replaced with others. The new enzyme is 50 times more stable than the wild-type or natural enzyme in organic solvents such as dimethylformamide. Further, under those conditions, it shows insignificant "amidase" activity, and thus can not degrade polyamides. It does however, retain "esterase" activity and can polymerize ester derivatives of amino acids to make polyamides containing as many as 50 monomers.

The CAM group also designed a new reagent, (MCS), methyl(β-cinnamoyl) sulfonate (Figure a). It is structurally similar to the natural substrate for subtilisin (Figure b) but does carry an activated methyl ($-CH_3$) group which it is able to transfer to the enzyme. This modification, like the use of DMA, results in a disproportionate degradation of amidase activity relative to esterase activity under the appropriate conditions.

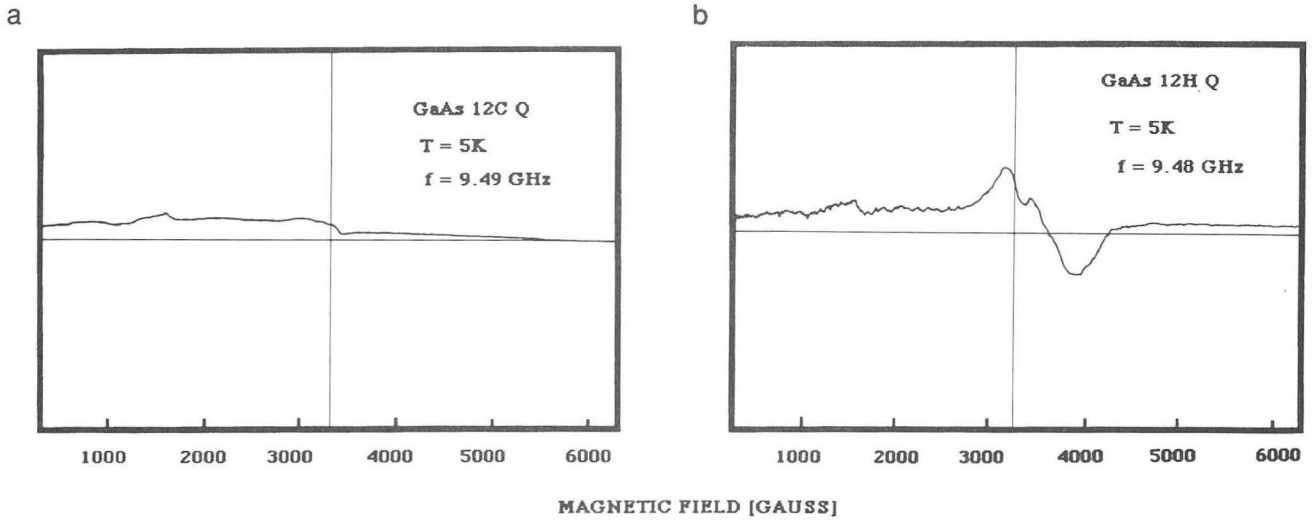
These results further support the concept of forcing normally degradative enzymes to create polymers and of using protein engineering as a viable route to the synthesis of polymeric materials. Detailed knowledge of the structure and function of enzymes can allow the rational redesign of the enzyme active site and thereby alter the functioning of the enzyme. This, along with the ability to alter the substrate specificity of enzymes, (see Research Notes 1/1), should allow the production of novel polymeric materials with interesting and important properties.

Bibbs, J.A., and C.H. Wong, "Selective Methylation of Subtilisin-His57 for Use in Controlled Synthesis," *J. Am. Chem. Soc.*, (in preparation).

Chen, S.T., J. A. Bibbs, W.J. Hemmen, Y.F. Wang, J. Liu, C.-H. Wong, M.W. Pantoliano, M. Whitlow, and P.N. Bryan, "Enzymes in Organic Synthesis: Use of Subtilisin and a Highly Stable Mutant Derived from Mutations," *J. Am. Chem. Soc.*, (in press).

Enzymatic Synthesis of Materials Project: Mark Alper, Project Leader (415) 486-6581; C.H. Wong (619) 554-4487; J.A. Bibbs (619) 554-3479.

Additional funding from the Division of Energy Biosciences, U.S. Department of Energy.



Electron paramagnetic resonance spectra of semi-insulating GaAs samples. Material in (a) shows good device performance. Devices on material in (b) show large diode leakage currents. The peak shown in Figure b is characteristic of the BE 1 defect. XBL 899-3482

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CAM *RESEARCH NOTE*

ELECTRONIC MATERIALS

DETRIMENTAL ROLE OF THE BE 1 DEFECT IN GaAs DETERMINED

Semi-insulating GaAs is an important semiconductor material for high-speed digital devices to be used in applications such as the next generation of supercomputers. The development of these devices is, however, severely hampered by materials problems, which are due, in part, to difficulties in controlling the defect incorporation during crystal growth and post-growth processing.

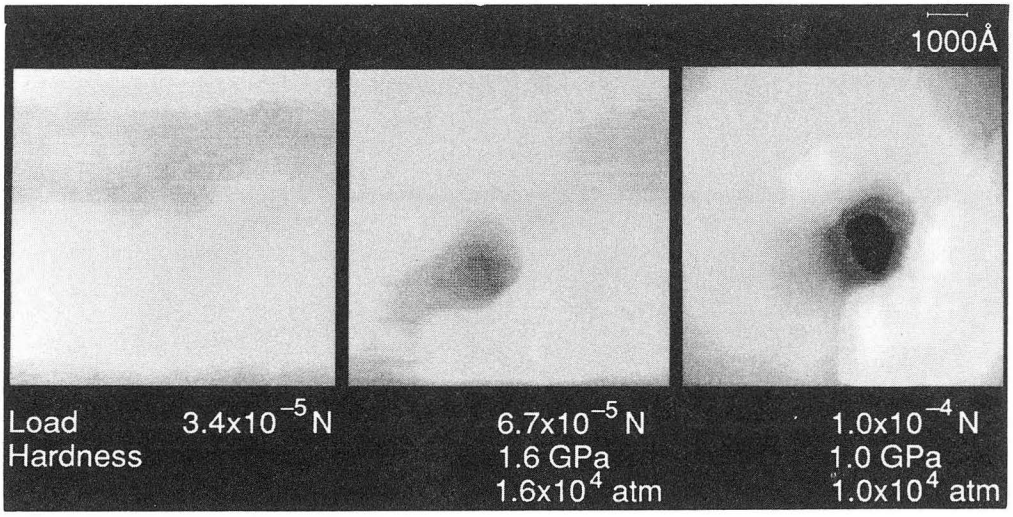
CAM scientists, under the direction of Eicke R. Weber, using electron paramagnetic resonance along with other optical and electrical characterization techniques, recently detected a new defect in undoped semi-insulating GaAs from a variety of commercial sources in the U.S., Japan, and West Germany. This defect, which they labeled "BE 1" (Figure 1), occurs unpredictably in state-of-the-art GaAs in concentrations which appear to be a function of both position in the single crystal boule and also the thermal history of the boule. High cooling rates result in high defect concentrations, while annealing at temperatures above 500°C followed by slow cooling can eliminate the defect.

The microscopic identity of GaAs-BE 1 has not yet been established; however a V_{Ga}-V_{As} divacancy is one of the possibilities considered. Its influence on device performance was investigated in collaboration with Reiner Zuleeg at McDonnell-Douglas. Comparing semi-insulating GaAs from various sources, a direct correlation between high concentrations of BE 1 and high leakage currents of diodes fabricated on the GaAs wafer could be established. Thus BE 1 can be identified as an electrically active center. Continuing research is focused on understanding the mechanism of BE1 in device failure and on other techniques to eliminate its occurrence.

Weber, E.R., and P. Omling, "Antisite Defects and El2 in GaAs," in *Festkörperprobleme/Advances in Solid State Physics XXV*, R. Grosse, editor, pp. 623, 1985.

Hoinkis, M., and E.R. Weber, "The GaAs-BE 1 Defect," in *Semi-Insulating III-V Materials*, G. Grossmann and L. Ledebo, eds., pp. 43, 1988.

Semiconductors Project: Eugene Haller, Project Leader, (415) 486-5294; Eicke Weber, (415) 642-0205.



Topographic images of gold films on mica that have been subjected to microindentation with increasing force (a-c). Height is represented as a color change (white is high, black is low). The surface before indentation was atomically smooth over the entire region. XBB 897-5542

Center for Advanced Materials

CAM *RESEARCH NOTE*

SURFACE SCIENCE AND CATALYSIS

ELASTIC AND PLASTIC DEFORMATION OF GOLD OBSERVED THROUGH ATOMIC FORCE MICROSCOPY

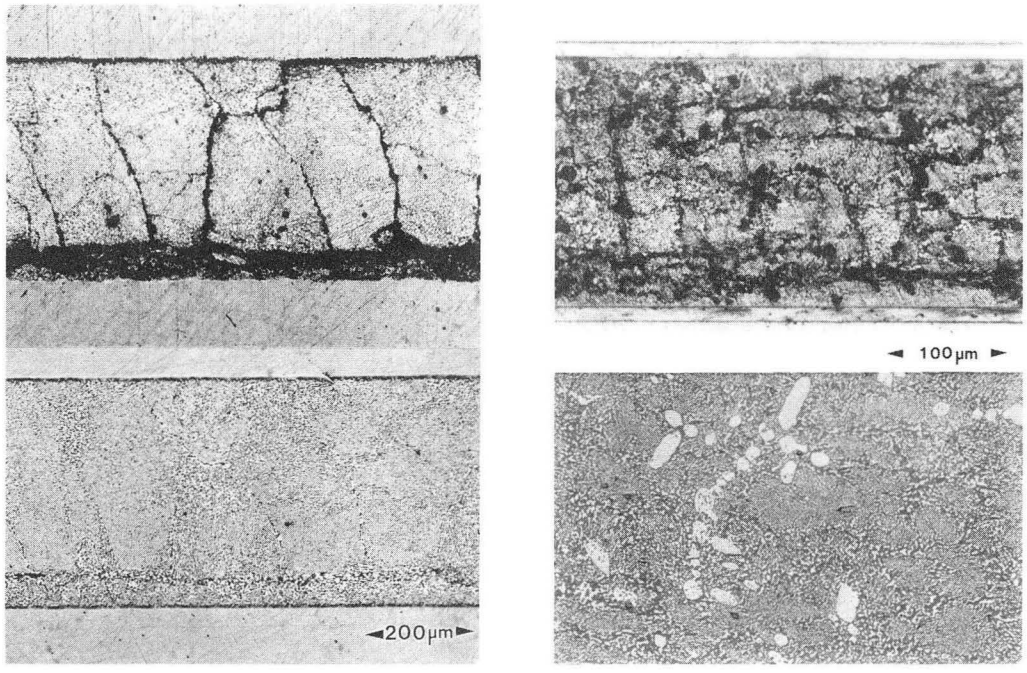
Whenever two surfaces come into contact the macroscopic behavior is determined by the atomic-level forces acting at each of the contact points. Deformation, wear, and friction all occur through the interactions occurring at these small asperities. Until now the unavailability of tools with sufficient spatial and force sensitivities has prevented the investigation of details of these processes. The newly developed Atomic Force Microscope (AFM) is, however, capable of sensing forces as low as 10^{-10} Newtons with atomic spatial resolution and can thus help to begin to explore these phenomena.

The AFM borrows from the technology of the Scanning Tunneling Microscope, but instead of measuring current, it measures the deflection of a small lever in response to the forces between the atoms of the substrate and those at the tip of the lever. It can be used to image the surfaces of metals, ceramics, plastics, and even liquids. It thus provides a window to the investigation of the mechanical properties of materials on an atomic scale.

CAM scientists, under the direction of G.A. Somorjai, in collaboration with G. Blackman at IBM Almaden Research Center, have used an AFM to study the initial stages of the mechanical deformation of thin films of gold evaporated on mica. The gold surfaces were imaged by scanning a diamond tip across them while keeping the force at a constant low value of ~10^{-10} Newtons, about 1% of the typical chemical bond strength. Then the tip was thrust into the surface with a force of 10^{-7} to 10^{-4} Newtons and the surface scanned again. When a load of up to about 2×10^{-5} Newtons was applied, only elastic deformation occurred and there was no detectable damage. However, at a load of 3.4×10^{-5} Newtons, a 1nm deep hole was produced, the result of plastic deformation (Figure 1a). As higher loads were applied, (Figures 1b and 1c), larger and deeper holes were produced. From these results the hardness (the load divided by the cross sectional area) of the surface of the gold film was calculated to be 1.6 GPa (the bulk value is 0.5 GPa). Continuing studies involve investigations of related phenomena including the viscoelastic deformation of polymers and the brittle deformation of ceramics.

Blackman, G.S., G.A. Somorjai, C.M. Mate, and M.R. Philpott, "Microindentation Studies with the Atomic Force Microscope," in preparation.

Surface Science and Catalysis Program, Gabor A. Somorjai, Program Leader, (415) 642-4053; Greg Blackman and M. R. Philpott, (408) 927-2223, (IBM Almaden Research Center San Jose, CA).



Deformation pattern (top) and polished microstructure (bottom) of a eutectic Pb-Sn solder joint (a) and a 58-Sn-40Pb-2In solder joint (b) deformed under shear creep conditions. In the binary material, the deformation is highly localized and occurs primarily parallel to the substrate (Cu) solder interface, along the direction of maximum shear. Close inspection of the polished joint microstructure reveals that the eutectic material has recrystallized and coarsened in the areas experiencing the greatest deformation. In the ternary material, the deformation is more homogeneous and the polished surface shows no microstructural changes.
XBB 887-7084, XBB 889-8164

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CAM *RESEARCH NOTE*

HIGH PERFORMANCE METALS

INDIUM AND CADMIUM ADDITION IMPROVES MECHANICAL PROPERTIES OF SOLDERS FOR ELECTRONICS APPLICATIONS

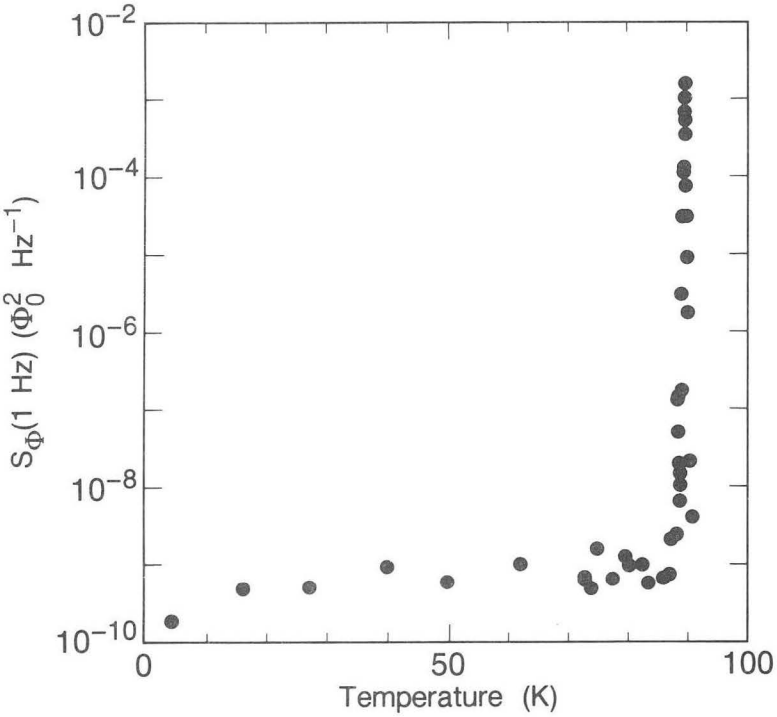
A solder contact in an electronic device commonly joins materials of different thermal expansion characteristics. Cyclic temperature changes, such as those routinely encountered during device operation, cause fatigue of the solder joint, ultimately causing its failure. This fatigue failure has been shown to arise from the inherent instability with respect to recrystallization of the as-solidified Pb-Sn solder microstructure and its tendency toward heterogeneous deformation when sheared. Thus the critical need in the design of new, more fatigue resistant solder alloys is the development of a solder that deforms more homogeneously in shear and once deformed, has a limited rate of recrystallization.

CAM researchers, under the direction of J.W. Morris, Jr., have recently shown that the deformation behavior and associated microstructural instabilities of solders can be altered through the addition of indium or cadmium to the near eutectic Pb-Sn mix. The investigation was conducted on experimental Pb-Sn solder joints, designed at CAM for testing in shear. The solder joints were deformed over a range of temperatures under creep conditions. Microstructural analyses of these joints in both as-deformed and polished states revealed that compared to the simple binary near-eutectic Pb-Sn solders, samples of the composition 58Sn-40Pb-2In and 58Sn-40Pb-2Cd exhibit significantly more homogeneous deformation behavior, and deform without a recrystallization of the eutectic material. Continuing work includes an evaluation of these ternary solders under thermal fatigue conditions.

Tribula, D., D. Grivas, D.R. Frear, and J.W. Morris, Jr., "Observations on the Mechanisms of Fatigue in Eutectic Pb-Sn Solder Joints," *J. Elect. Packag.*, June 1989, 111, 83.

Tribula, D., and J.W. Morris, Jr., "Creep in Shear of Experimental Solder Joints," to be presented at the annual ASME Conference, San Francisco, California, December 1989, to be published *J. Elect. Packag.*.

Solders Project: J.W. Morris, Jr., Project Leader (415) 642-3815; D. Tribula, (415) 486-4526.



Spectral density of noise in YBCO film as a function of temperature. Notice the small increase in the noise from 4.2 K to above 80 K. XBL 895-5125

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CAM *RESEARCH NOTE*

HIGH-T_C SUPERCONDUCTIVITY

LOW MAGNETIC FLUX NOISE OBSERVED IN THIN FILMS OF YBCO

The lowest level of low-frequency magnetic flux noise yet reported in a high-temperature superconductor at 77 K has been observed in a pulsed laser deposited thin film of $YBa_2Cu_3O_{7-\delta}$ (YBCO). The measurements, performed by CAM scientists J. Clarke, M.J. Ferrari, M. Johnson, and F.C. Wellstood were made in a specially designed cryostat in which the film sample, whose temperature could be varied from 4.2 K to above its transition temperature (T_C), of 90 K was placed about 100 μm from a niobium-based dc SQUID (Superconducting QUantum Interference Device) maintained at 4.2 K. The magnetic noise generated by the film, which arises from the thermally activated motion of flux vortices pinned in the material, is detected by the SQUID.

Results obtained using films produced at Bellcore and Rutgers University by A. Inam, X.D. Wu, L. Nazar, and T. Venkatesan show that the spectral density of the noise scales with the inverse of the frequency (1/f) and increases slowly with temperature from 4.2 K to just below T_C, where it exhibits a sharp peak (Figure 1). The "1/f" noise level measured is low enough to suggest that it may be possible to produce dc SQUIDs for most practical applications requiring operation at 77 K. In fact, the 1/f flux noise measured in the YBCO film at 77 K is within a factor of five of that produced by the only commercially available niobium-based dc SQUID operated at 4.2 K.

The results demonstrate that a high degree of crystalline orientation and surface smoothness as well as high critical current densities will be required for films used in SQUIDs and in flux transformers coupled to SQUIDs to produce magnetometers or magnetic gradiometers.

M.J. Ferrari, M. Johnson, F.C. Wellstood, J. Clarke, A. Inam, X.D. Wu, L. Nazar, and T. Venkatesan, "Low Magnetic Flux Noise Observed in Laser-Deposited *in situ* Films of $YBa_2Cu_3O_{7-\delta}$ and Implications for High-T_c SQUIDs," *Nature*, (in press).

Center for Thin Film Applications: John Clarke, Project Leader, (415) 642-0330; M.J. Ferrari, M. Johnson, (415) 642-3634; F.C. Wellstood, (415) 642-3069; L. Nazar and T. Venkatesan, Bellcore; A. Inam and X.D. Wu, Rutgers University.

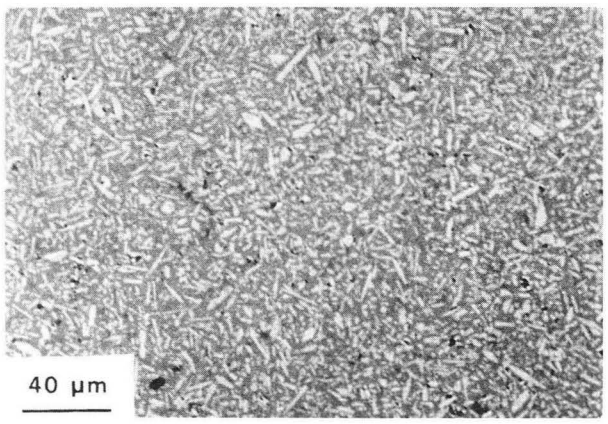

Figure 1
Polished surface of hot-pressed alumina-coated SiC whiskers showing uniform distribution of SiC whiskers (light grey phase). This surface is perpendicular to the hot pressing direction. XBB 890-7086

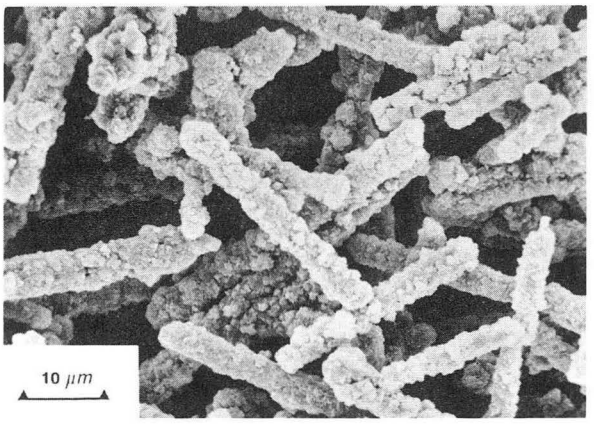

Figure 2
Alumina-coated SiC whiskers. These whiskers, originally with diameters ranging from 0.25-3µm, have been fully coated, preventing direct whisker contacts in the green body. This enhances densification and provides a more uniform distribution of the whiskers in the composite. XBB 894-3077

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CAM *RESEARCH NOTE*

CERAMIC SCIENCE

NOVEL PROCESSING METHOD DEVELOPED FOR ALUMINA-SiC WHISKER COMPOSITE

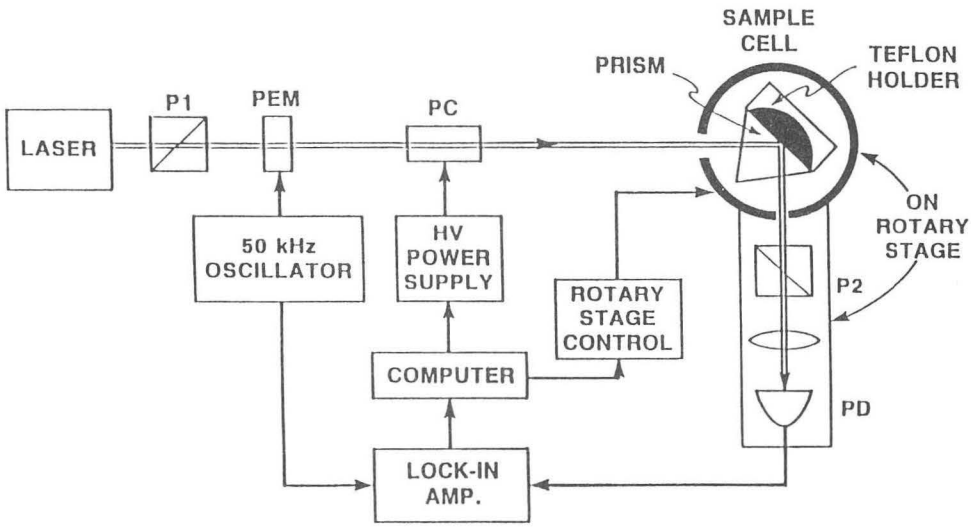
Researchers in the CAM Ceramic Science Program have developed a method for coating SiC whiskers with thick layers of a polycrystalline alumina precursor. The resulting composite powders are used to produce alumina/SiC composites for use in applications such as ceramic cutting tools.

The SiC whisker content in currently available alumina silicon carbide ceramic composites is limited to about 15 vol %. Further, these composites tend to contain whisker clusters, resulting from the difficulties inherent in mechanical mixing of powder and whiskers. These clusters degrade the mechanical properties of the composites greatly. The method developed here has produced dense composites with over 40 vol % of SiC, and whisker clustering is completely eliminated. Composites of high uniformity, and high volume fraction of whiskers can be obtained. An optical micrograph of a composite produced in this manner is shown in Figure 1.

The process involves the use of a slurry in which SiC whiskers, suspended in water, are coated in a controlled precipitation reaction depositing aluminum sulfate on the whisker surfaces only. The resulting composite powder is dried and calcined, and then hot pressed around 1600°C to full density. A micrograph of some coated whiskers is shown in Figure 2. A key element in the process is the use of an appropriate polymeric dispersant and the careful control of the precipitation reaction.

Continuing research is focused on the extension of this slurry coating method to produce barrier coatings on the whiskers, and on the role of various particle shapes and process variables in determining the mechanical properties of the dense composites. Initial testing by microindentation has shown a fracture toughness of between 8 and 10 $MPa \cdot m^{1/2}$ for the composites shown in Figure 1.

Ceramic Processing Project: Lutgard De Jonghe, Project Leader, (415) 486-6138; David Kapolnek, (415) 486-6138.



Schematic diagram of the experimental apparatus. P1 and P2 are polarizers, PEM is a photoelastic modulator, PC is a pockell cell, and PD is a Photo-diode. XBL 8910-3659

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CAM *RESEARCH NOTE*

SURFACE SCIENCE AND CATALYSIS

POLYMER CONCENTRATION PROFILE MEASURED BY EVANESCENT WAVE ELLIPSOMETRY

Polymer adsorption at a liquid/solid interface is a problem of great importance in technological areas such as painting and coating. In the past, x-ray fluorescence and optical evanescent fluorescence techniques have been used for the study of how polymer adsorption and depletion (non-sticking) at a liquid/solid interface depends on various parameters such as polymer composition, molecular weight, solvent quality, and ionic strength. Recently, in collaboration with Industrial Fellow M.W. Kim of Exxon Research and Development, and D.G. Peiffer, also of Exxon, an evanescent ellipsometry technique for such studies was developed.

This phase modulated technique has a submonolayer sensitivity which allows the non-destructive measurements of adsorption and depletion profiles of polymers in solution near a solid interface. In comparison to other techniques, there is no need to chemically modify the polymer structure in order to enhance its x-ray or light fluorescence capability and the probing depth can be reduced to the order of an optical wavelength, thus allowing the measurements to be easily performed *in-situ*.

The technique has been successfully applied to the adsorption case of Mn-neutralized sulfonated polystyrene on glass from dimethylsulfoxide solution and the depletion case of polystyrene on glass from ethyl acetate solution. The characteristic lengths of the adsorption and depletion layers were deduced and were found to be close to the molecular dimensions of the polymer coils in the two solvents respectively.

Continuing work will involve the investigation of the transition from depletion to adsorption of polymers by varying the amount of metal-neutralized sulfonated groups chemically bound to the polystyrene backbone or the surface treatment of the glass substrate. Studies of the dynamics of the adsorption or depletion process are also planned.

Kim, M.W., D.G. Peiffer, W. Chen, H. Hsiung, Th. Rasing, and Y.R. Shen, "Polymer Concentration Profile Near a Liquid/Solid Interface: Evanescent Wave Ellipsometry Study," *Macromolecules*, 22, 2682, 1989.

Instrumentation for Surface Science Project: Y.Ron Shen, Acting Project Leader, (415) 642-4856; Mahn Won Kim and D.G. Peiffer, Exxon Research and Development, (201) 730-2863; Wei Chen, (415) 642-1107.

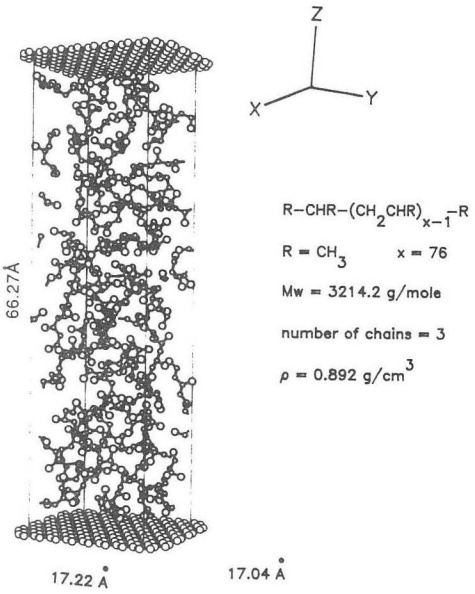

Figure 1 (right)
An atomistic model was developed to explore the structure and mechanical properties of an amorphous glassy polymer adsorbed onto a graphite surface. The predicted structure is periodic in the x and y directions and, in this simulation, two graphite basal planes are shown, one at the top and one at the bottom of the z axis. Three polymer chains are present, each of molecular weight 3214. Ensembles of such structures, in a state of mechanical equilibrium, are useful in providing quantitative molecular based information on the properties of composite interfaces.
(XBL 8910-3658)

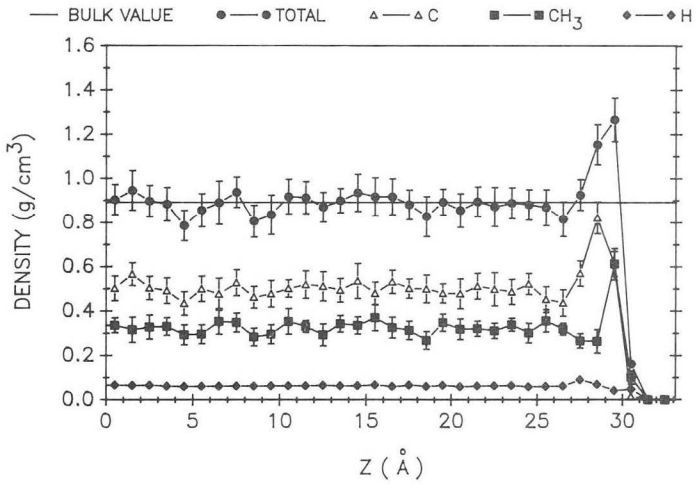

Figure 2 (left)
Local mass density distribution at a glassy polymer/graphite interface. The centers of carbon atoms of the graphite surface are located at z=33.1Å, and the region near z=0 is representative of unperturbed bulk polymer. The solid line represents the experimentally observed macroscopic density at the simulation temperature (20°C below T_g). Individual contributions to the mass density display a strong maximum next to the highly attractive surface. Chains adsorb on the surface through their pendant groups. (Note that peak density of -CH_3 groups is closer to graphite surface than peak density of carbons of polymer backbone.) (XBL 8910-3660)

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CAM *RESEARCH NOTE*

POLYMERS AND COMPOSITES

PREDICTION OF STRUCTURE AND ADHESION AT A GLASSY POLYMER/SOLID INTERFACE

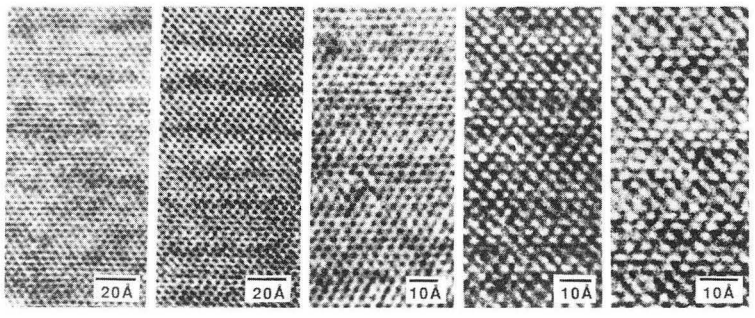
The thermodynamic and mechanical properties of amorphous polymers adhering to solid substrates are relevant in many applications. The performance of adhesives and coatings, such as the resists used by the microelectronics industry, and the interactions between the matrix and filler in advanced composite materials are important examples. It is therefore highly desirable to quantitatively relate interfacial behavior to the fundamental chemical constitution of these polymer/solid systems. The principles of statistical mechanics provide a link between interactions at the atomic level and macroscopic properties; their implementation to systems as complex as glassy polymer/solid interfaces constitutes a major challenge.

CAM researchers under the direction of D.N. Theodorou have developed a computer simulation approach for the accurate prediction of interfacial structure and mechanical performance of a glassy polymer (atactic polypropylene) adhering to a graphite surface. The method rests on generating an ensemble of atomistically detailed multichain microstructures. Each microstructure is relaxed to a state of mechanical equilibrium by an energy minimization technique on a Cray X-MP/48 supercomputer. The work of adhesion, estimated from interatomic forces and distances in the model microstructure without any adjustable parameters, was predicted to within 13% of experiment. In addition, the details of chain organization and conformation at the interface have been elucidated: local segment density is enhanced, and bond orientation deviates from isotropy over a 10Å-thick region near the graphite. Chains adsorb on the graphite through their pendant methyl and hydrogen groups. There is a distinct tendency for adsorbed hydrogens to locate themselves preferentially over the centers of hexagons in the graphite honeycomb. Chain segment clouds orient with their longest principal axis parallel to the solid substrate. Local structure assumes its bulk characteristics at distances larger than two chain radii of gyration from the graphite surface. In continuing work, these model microstructures will be subjected to shear deformation in order to explore the mechanisms of interfacial failure between polymer and solid.

Mansfield, K.F., and D.N. Theodorou, "Atomistic Simulation of a Glassy Polymer Surface," submitted to *Macromolecules.*

Mansfield, K.F., and D.N. Theodorou, "Molecular Modeling of Polymers at Interfaces," *Polym. Prepr., Am. Chem. Soc., Div. Polym. Chem.*, vol. 30, p. 76, 1989.

Polymer Substrate Interactions Project: Doros N. Theodorou, Project Leader (415) 643-8523; Kevin M. Mansfield, (415) 642-5927.



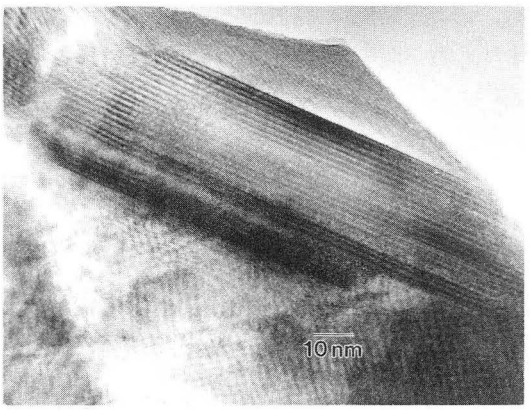


Figure 1 (left)
High-resolution TEM images of BCSCO in [001] orientation. Materials from left to right: undoped, Fe-doped, Ni-doped, Co-doped, Ga-doped. XBB 894-3086A

Figure 2 (right)
In Fe-doped specimens, high-angle grain boundaries shown here occur frequently. This type of grain boundary has not been seen with the other dopants, or in the undoped material. Therefore, its presence in the Fe-doped specimens suggests that introduction of Fe must cause some change in the surface energy, and hence microstructure, of the material. It is known that the preferred three-fold oxygen coordination of Fe enhances twin formation in the Fe-doped $YBa_2Cu_3O_z$ and it is possible that a similar mechanism is inducing high angle boundaries of the type shown here. XBB 894-3088

Center for Advanced Materials

CAM *RESEARCH NOTE*

HIGH-T_c SUPERCONDUCTIVITY

STRUCTURE/PROPERTIES RELATIONSHIP IN DOPED SUPERCONDUCTORS EXPLORED WITH HIGH RESOLUTION TEM

Resistivity data from the Texas Center for Superconductivity at the University of Houston have shown that the superconducting transition temperature is lowered significantly in Fe- and Co-doped BiCaSrCuO, but only marginally in Ni and Ga doped material. Although the four dopant species are all thought to substitute for copper in the BCSCO crystal structure, little is known about the correlation between any microstructure changes that might result from the doping and the observed changes in superconducting properties.

CAM scientists R. Gronsky, M. Fendorf, K. Fortunati, and C. P. Burmester, at LBL's Center for Electron Microscopy have used high-resolution transmission electron microscopy (TEM) techniques to examine these relationships. Although TEM results obtained and computer-enhanced to obtain maximum detail showed no difference in crystal structure between doped and undoped materials (Figure 1), changes in microstructure were observed for the Fe-doped material. The grains in these samples appear to be smaller than those found in undoped material and rather than assuming the typical random crystallographic orientation, they appear to be perpendicular to the surrounding matrix (Figure 2). The grains also are seen to have an unusually high aspect-ratio.

It is surprising, however, that no microstructural changes seem to appear in the Co doped material, since its resistivity curve is very similar to that for the Fe-doped samples. This result, together with the absence of any observable crystallographic or microstructural changes in Ni-and Ga-doped specimens, suggest that variations in T_c are due primarily to electronic, rather than structural differences between doped and undoped materials. Thus, although the observed "texturing" of the grains and the resulting increased grain boundary area of the Fe- doped structure may cause some limited lowering of the superconducting transition temperature, the concomitant weak conduction links and flux pinning at grain boundaries might be expected to have a much more dramatic effect on properties, such as the critical current and critical magnetic field of the superconducting material.

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High T_c Superconductivity Program, Norman E. Phillips, Program Leader, (415) 486-6062; Ronald Gronsky, (415) 486-5674; Mark Fendorf, Kim Fortunati, and Chris P. Burmester, (415) 486-7361.

Research supported by DARPA through Texas Center for Superconductivity at the University of Houston, Grant No. MDA972-89-J-1001.

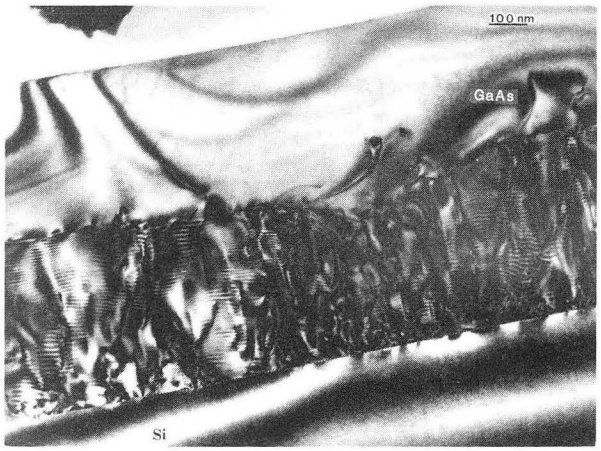

Figure 1
TEM cross-section micrograph of the GaAs/Si interface with 50 periods of InGaAs (25% In)/GaAs strained layer superlatices (SLSL) grown directly at the interface with Si. Note the large number of stacking faults formed at the interface, propagating through the SLSL and stopping at the last interface with epilayer of GaAs. Bending of dislocations was most effective at this interface. XBB 871-46

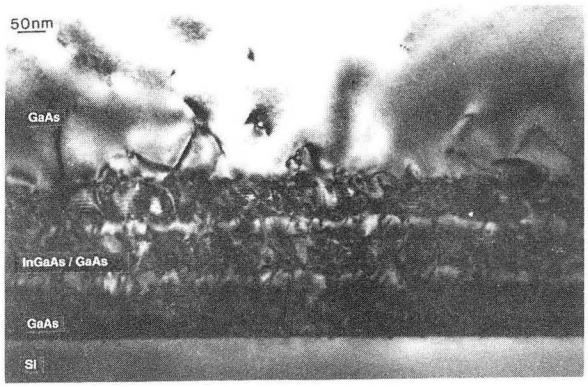

Figure 2
TEM micrograph of the GaAs/Si interface with the application of three *packages* of ten periods each of the InGaAs/GaAs SLSL. Note dislocation bending at each package interface. Occasionally, the formation of new dislocation was observed. Application of *packages* of SLSL was most successful in decreasing dislocation density in the epilayer. XBB 874-3060

Center for Advanced Materials

CAM *RESEARCH NOTE*

ELECTRONIC MATERIALS

TECHNIQUE DEVELOPED TO REDUCE DEFECT DENSITY IN GaAs LAYERS GROWN ON Si

The promise of integrating GaAs optoelectronics with Si digital devices in applications such as optical interconnects is clouded by the fact that differences in lattice parameters and thermal expansion coefficients between the two materials lead to high defect density ($\sim 10^{11}/cm^2$) in the GaAs epilayer.

CAM scientists under the direction of J. Washburn, in collaboration with H. Kreomer's film growing group at the University of California, Santa Barbara, have shown by cross-sectional TEM that defect propagation into the epitaxial GaAs layer can be effectively decreased by initial growth of strained layer superlattices (SLSL) such as GaAs/InGaAs between the silicon and final epitaxial GaAs layer (Figure 1). It was found that the number of GaAs/InGaAs periods did not influence the reduction of dislocations propagating into the final GaAs film once a minimum number, dependent on the composition of the InGaAs was deposited. The upper interface between SLSL and the final GaAs layer is however, most efficient in dislocation bending, preventing the extension of the defect to the critical, uppermost layer of GaAs. By growing three "packages" (Figure 2) of ten periods of SLSL measuring 10 nm each (a process that creates three such upper interfaces), a density of dislocation as low as $2 \times 10^7/cm^2$ was obtained. Other defect reduction mechanisms are being investigated.

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High Performance Metals Program

Metals for Advanced Applications Project

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