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Physical and Chemical Sciences Center

F. L. Vook, Director

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Research Briefs

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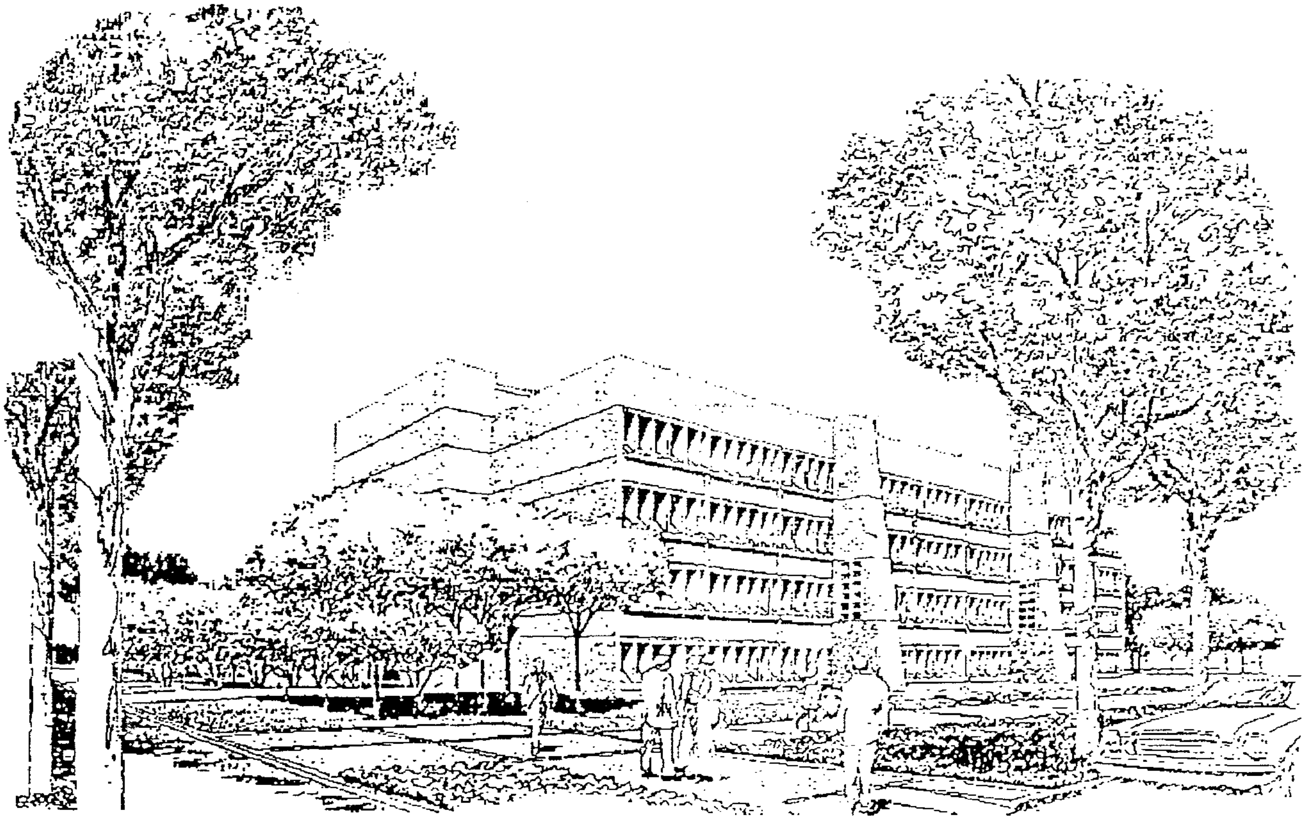

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Physical and Chemical Sciences Center
Research Briefs

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Message from the Director

As Sandia National Laboratories and the Physical and Chemical Sciences Center develop an increasingly diverse set of customers, research partners, and Cooperative Research and Development Agreements (CRADA's) with industry, there is a need for providing more concise information describing our technical achievements and capabilities. This publication, *Research Briefs,* is designed to inform our present and potential partners in research and technology advancement.

Our research emphasizes semiconductor physics, electronic materials, surface physics and chemistry, plasma and chemical processing sciences, lasers and optics, vision science, ion-solid interactions and defect physics, and advanced materials physics. The specific programs we pursue are driven by our research goals which are greatly influenced by interactions with our government and industrial customers.

People are our most important asset and their creative research is fundamental to our accomplishments. Leadership, teamwork, and individual innovation are the strengths we use to help Sandia respond to the present and future needs of our country.

Frederick L. Vook

Frederick L. Vook
Director

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Research Briefs

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Interfacial-Force Microscopy Probes the Mechanical Properties of a Single, Nanometer-Size Grain

by J. E. Houston and T. A. Michalske

Motivation — Considerable excitement has recently been generated in the potential for creating unique materials that are constructed from nanometer-size building blocks—the so-called "nanophase materials." Such materials show promise of being stronger, lighter, more resistant to hostile environments, and easier to form into complex shapes. However, in obtaining an understanding of the role of the small building blocks in improving materials properties, it is necessary to be able to make mechanical measurements on this same dimensional scale. The newly developed interfacial force microscope (IFM), which was developed under our BES/MS "Fundamental Science of Adhesion" program, is ideally suited for such a purpose. This technique is capable of measuring the force to break a single bond in a molecule and can determine position to less than an atomic diameter. These capabilities permit the determination of the mechanical properties (for example, elasticity, inter granular motion, threshold for plasticity, and the defect mode of plastic deformation) of a single grain in these unique materials.

Accomplishment — We have applied the IFM to the first study of the mechanical behavior of individual grains in polycrystalline Au films deposited on glass substrates. The tungsten scanning-force probe has a nanometer scale tip and can be rastered across the surface to produce repulsive force images. An example of such an image is shown in the accompanying figure. In addition, the probe can be ramped into surface contact to measure the interfacial force necessary to produce local deformation (loading curves). By a detailed analysis of scanning-force images and loading curves, we can obtain quantitative values for the modulus of elasticity and shear-stress threshold for plastic (or permanent) deformation of individual grains. These measurements are made possible by the unique capabilities of the self-balancing force sensor used in the IFM. No present scanning force microscopy or conventional nanoindentation instrument employs this unique sensor design which allows stable, quantitative interfacial force measurements without the mechanical instabilities. Our single-grain analyses for these particular samples yields values for the elastic modulus of 66 GPa and a shear-stress threshold of 2.6 GPa for gold.

Significance — Measurements such as these will permit an accurate evaluation of the mechanical properties for nanophase materials as a function of the details of the fabrication processing. This, along with modeling, will permit fabrication to be fined tuned to tailor materials for specific applications. A CRADA with Digital Instruments, AT&T, and the University of New Mexico is in place to commercialize this unique materials probe.

Keywords: nanophase materials, scanning probe microscopies, force sensors

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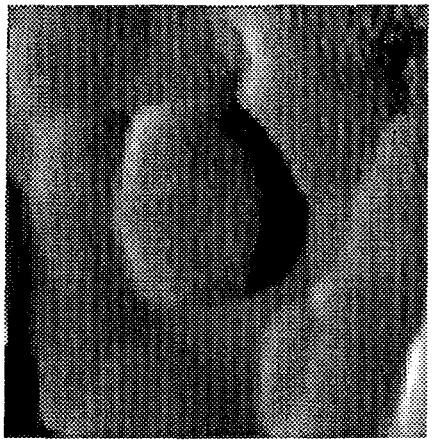

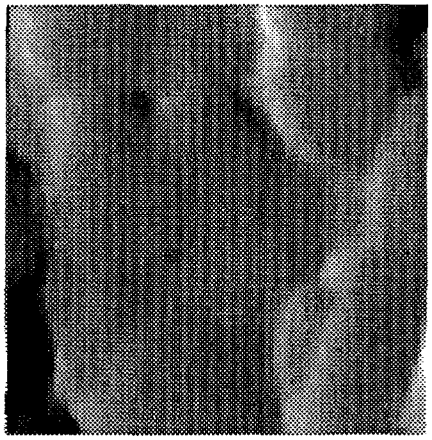

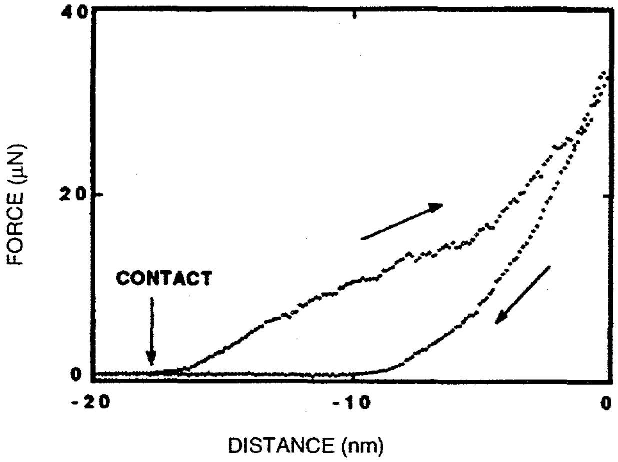

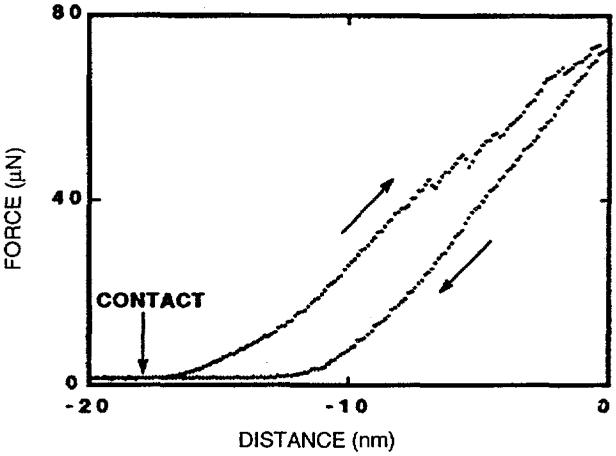

The image shown at the top left represents a 400x400 nm portion of a 200 nm thick Au film deposited on a glass surface. The surface consists principally of large, flat 200 nm diameter grains with an occasional grain protruding from the normal surface by about 10 nm (the large grain in the center of the left-hand image above). By ramping the probe into the center of this grain and then withdrawing it from the surface, we generate the loading profile shown in the bottom left-hand plot. The loop in this plot indicates a permanent deformation of the surface. The center image shows that the observed loading profile corresponds to a sliding of the entire grain with respect to its neighbors. This grain was not in contact with the glass substrate and loading pushed it down into rigid contact. The plot at the bottom right shows the loading profile for the same grain while in contact with the underlying substrate indicating a further permanent deformation of about 4 nm. The image at the far right shows that the latter deformation was experienced within the grain itself. Images and loading-cycle data combinations such as these allow for the first time the determination not only of quantitative values for various mechanical variables but also provides a basic understanding of the root causes of the behavior; for example, grain-boundary motion, indentation, defect creation, etc.

New Heavy-ion-backscattering Technique extends Sensitivity of Ion Beam Analysis by Orders of Magnitude

by **J. A. Knapp and J. C. Banks**

Motivation — For many new problems in materials research, especially for contamination control in microelectronics, very high sensitivity to surface impurities is required. Indeed, by the turn of the century, advanced generations of microelectronics will require metal contaminants to be kept well below 1×10^9 atoms/cm^2 on the surfaces of wafers. These levels are well below the detection limits for **all** existing surface analyses, including Total reflection X-Ray Fluorescence spectroscopy (TXRF), an X-ray technique now commonly used in microelectronics. Because of Sandia's unique capabilities and expertise in all types of ion beam analyses, we have been addressing this need for extreme surface sensitivity with a new approach to ion backscattering spectrometry which is far more sensitive than previous ion beam techniques.

Accomplishment — The approach we have developed uses backscattering of moderate energy (a few hundred keV) and heavy ions for increased sensitivity. The technique is called Heavy Ion Backscattering Spectrometry (HIBS) and has already demonstrated sensitivity for medium-to-heavy surface impurities on Si, more than 1000x greater than conventional Rutherford Backscattering Spectrometry (RBS). Background due to overlapping counts from the substrate, a major problem, is eliminated by a thin, self-supporting foil in front of the detector; ranging out lower-energy ions scattered from the substrate and allowing only higher-energy ions scattered from impurities heavier than the substrate to reach the detector. Using 100-200 keV N^+ beams and time-of-flight ion energy detectors, we expect to reach sensitivities of 5×10^9 atoms/cm^2 for Fe and 1×10^8 atoms/cm^2 for Au on a Si substrate. The figure shows the sensitivity as a function of the impurity atomic number for HIBS and for TXRF, the best competing technology applicable to surface analysis.

Significance — The potential of HIBS for extremely sensitive trace-element analysis has been recognized in several ways, including a U.S. patent, an LDRD for development of advanced HIBS detector technology, and as part of a BES/MS award for "Sustained Outstanding Research" recognizing Sandia's ion beam analysis expertise. Under a CRADA, SEMATECH is funding a prototype stand-alone HIBS system with dedicated accelerator and chamber. This system will be sited at Sandia and serve as a user facility for Sandians and SEMATECH member companies for wafer contamination studies and research to minimize such contamination.

Keywords: microelectronics, ultra-trace contamination detection, ion beam analysis, heavy ion backscattering spectrometry

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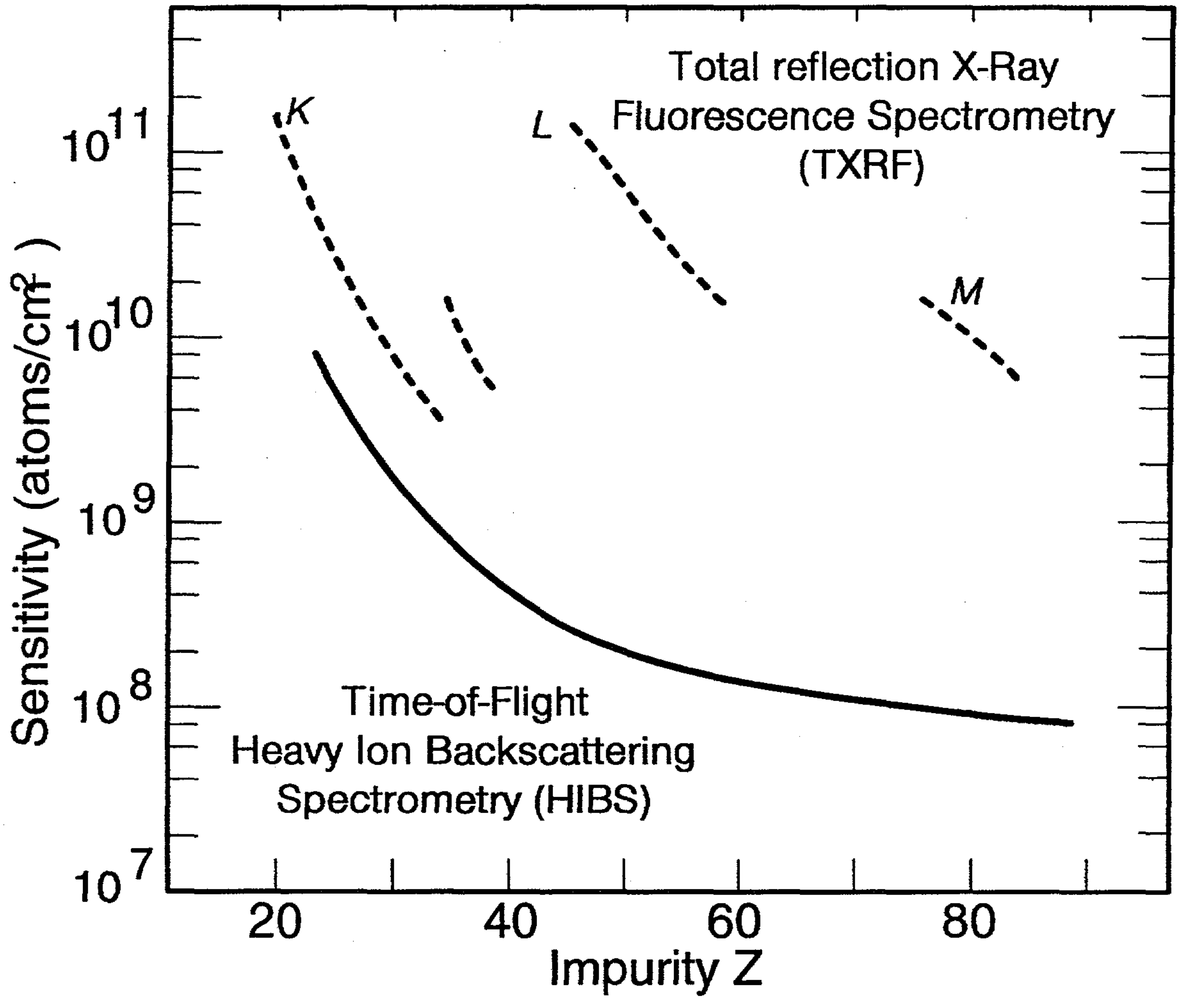
Detection limits for heavy ion backscattering are much lower than for other techniques.



Detection limits for Heavy Ion Backscattering Spectrometry (HIBS) as a function of impurity atomic number, compared to the detection limits for Total reflection X-Ray Fluorescence (TXRF). The latter technique is commonly used for contamination control in microelectronic fabrication lines, and is the most sensitive commercially available surface analysis technique.

KMAP X-ray Diffraction Determines the Structure of Single-crystal Thin Films 100 Times Faster than Previously Possible

by **S. R. Lee and B. L. Doyle**

Motivation — Successful fabrication of III-V compound semiconductor devices requires well characterized materials produced by a reproducible, reliable growth process. Double-crystal rocking-curve analysis is often used to measure the lattice structure of single-crystal thin films and to determine the quality of III-V materials grown by various processes (MOCVD or MBE, for example). Rocking-curve analysis is a powerful tool when applied to low-strain or lattice-matched materials which are highly perfect, but many advanced materials of interest in optoelectronic applications are highly strained. Relaxation of strain produces microscopically and macroscopically tilted crystal domains within the highly-strained films which limit the effectiveness of rocking curve analysis. The complications introduced by tilting can be overcome by using a device called a triple-axis diffractometer — however, use of the triple-axis system increases the time for analysis from a few minutes to many hours.

Accomplishment — We have overcome the limitations of both standard rocking curve analysis and triple-axis diffractometry by developing a new x-ray diffraction technique (which we call "KMAP") for efficiently determining the structure of highly-strained, single-crystal, thin film materials. Our technique combines a traditional double-crystal x-ray diffractometer with a position-sensitive x-ray detector to rapidly map x-ray intensity in two dimensions — a typical intensity map is shown in the upper-left panel of the adjacent figure. The position-sensitive detector improves the double-crystal system by measuring the total scattering angle of diffracted x-rays in a parallel fashion. Measurement of this angle allows us to directly map the lattice structure and remove crystal tilting effects. Comparison of a traditional rocking curve (lower-left panel) and our KMAP results (upper-right panel) for a typical multilayer film shows the ability that KMAP has to directly resolve structure not observed using rocking curve analysis. This enhanced analysis of crystal structure is carried out in 100-1000 times faster than is possible with a serially-scanned, triple-axis diffractometer.

Significance — We have been applying KMAP to characterize a wide variety of advanced materials and solid-state devices produced at Sandia in order to understand and improve the processing of these materials. Analytical examples include the determination of lattice constants, strain, composition, epilayer tilting and mosaic spread of InAsSb/InSb superlattices and GaInSb buffer layers for photovoltaic detectors, InAlAs and InGaAs superlattices and buffer layers for optical modulators, ion-implanted and regrown SiGeC films for the study of band-gap engineering in Group IV materials, and anodically-produced porous Si films.

Keywords: compound semiconductors, x-ray diffraction, double-crystal rocking curve analysis, triple-axis diffractometer, reciprocal space, strain relaxation

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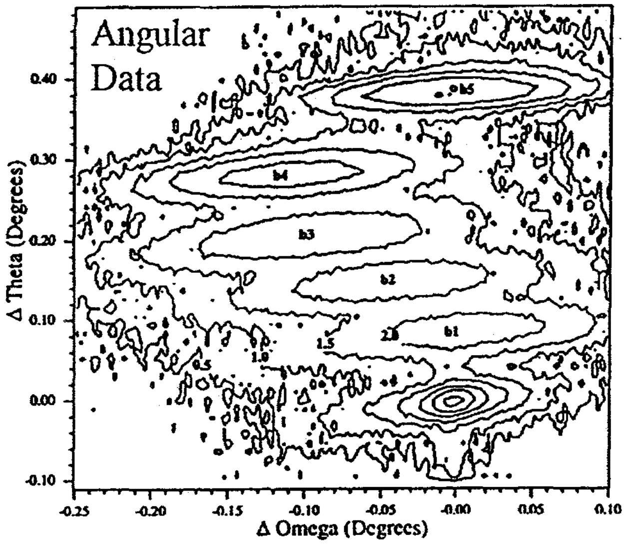
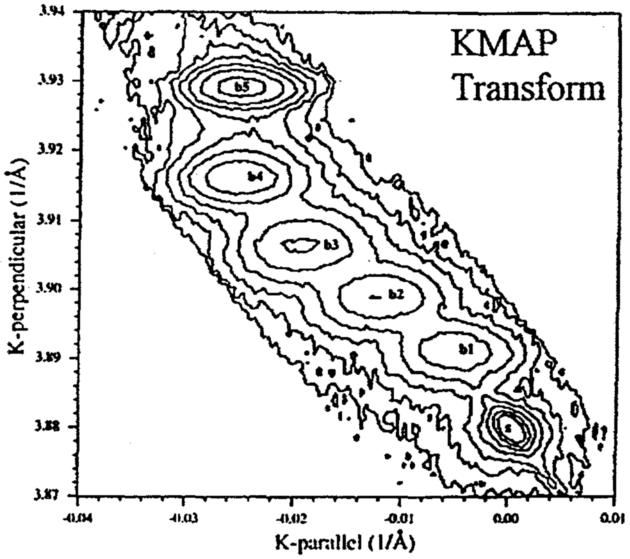
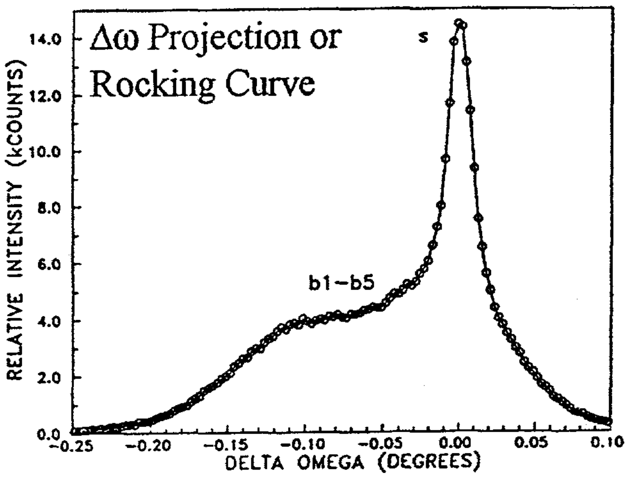
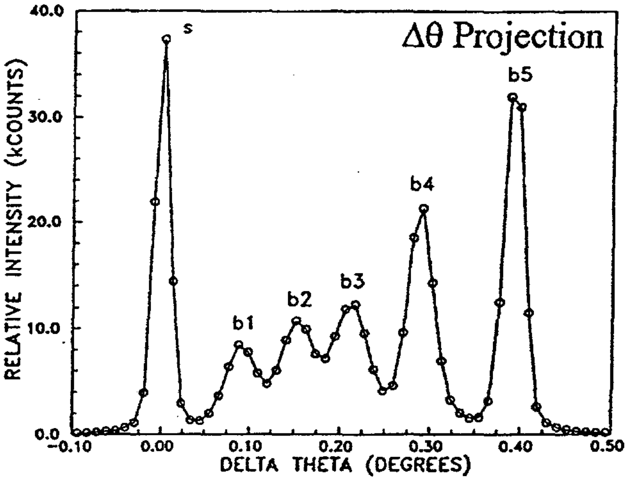
KMAP X-Ray Diffraction Analysis of a 5-Layer GaInSb Film Reveals Lattice Structure That Is Not Seen Using Rocking Curve Analysis.









KMAP x-ray diffraction analysis provides this enhanced analysis 100 times faster than its only competitor -- the traditional triple-axis diffractometer.

KMAP x-ray diffraction analysis is a relatively new technique invented within Center 1100. The technique directly measures the reciprocal space crystal structure of epitaxial layers. Density in reciprocal space is efficiently mapped by using a position-sensitive detector in place of the conventional x-ray detector on a standard double-crystal diffractometer. Use of the position-sensitive detector converts a double-crystal diffractometer into the functional equivalent of a triple-axis diffractometer with one very important difference -- the θ-2θ axis scan is now collected in a parallel fashion using the position sensitive-detector, instead of using the serial mechanical scanning required in a conventional triple-axis system. The net effect is a complete analysis of crystal structure in 10-30 minutes using KMAP instead of 10 hours or more using a conventional system.

A New Monitor Provides Non-destructive Measurement of Near-surface Tritium

by **W. R. Wampler**

Motivation — Early detection of tritium leaks in weapon systems is needed to insure the reliability and safety of the weapon. New methods to detect tritium contamination are also needed to reduce the risk of accidental release of tritium or exposure of workers to tritium during dismantling of weapons. The low energy of the betas emitted when tritium decays makes tritium especially difficult to detect compared to other radioisotopes. Conventional methods to detect tritium on surfaces usually require dissolving a wipe or a piece of material and liquid scintillation counting. This procedure has several disadvantages. It is costly and laborious and does not provide real-time information and it generates mixed waste. Furthermore, wipes only detect loosely bound tritium. Quantitative measurement of non-removable tritium by the dissolution method requires destruction of the object being tested which may not be desirable.

Accomplishment — A new way to measure tritium on surfaces has recently been developed which avoids these difficulties. The new method uses a PIN photodiode and low noise pulse amplifier to count tritium betas emitted from a surface. The method measures tritium surface contamination by placing the sensor against a surface to be tested and observing the count rate. A lower limit for detection of tritium activity of about 0.1 disintegration per second (~3×10^{-12} Curie) per square centimeter has been demonstrated.

Significance — Potential applications for the new tritium monitor extend beyond the defense program to the DOE's Magnetic Fusion Energy program where tritium is also used. The initial prototype of the monitor has been used to measure the amount of tritium on components from the Joint European Torus following recent tritium fueled plasma experiments (see illustration). A second version of the monitor, designed to measure tritium inside the vacuum vessel of the Tokamak Fusion Test Reactor, is currently undergoing tests at the Princeton Plasma Physics Laboratory. Since the tritium monitor consists entirely of electronic components, it can be made small and rugged for long term operation in a weapon system or storage container or at locations where access is restricted. Alternatively, it can be implemented as a hand-held unit to provide real-time non-destructive surveys during assembly or disassembly of components from weapons or fusion reactors. Since the potential exists for commercialization, a patent disclosure (DOE #78,022; SD-5231) has been filed on this new tritium monitor. A Focal Point Project for FY94 has been initiated to explore defense related applications of the monitor.

Keywords: tritium monitor, radiation detection

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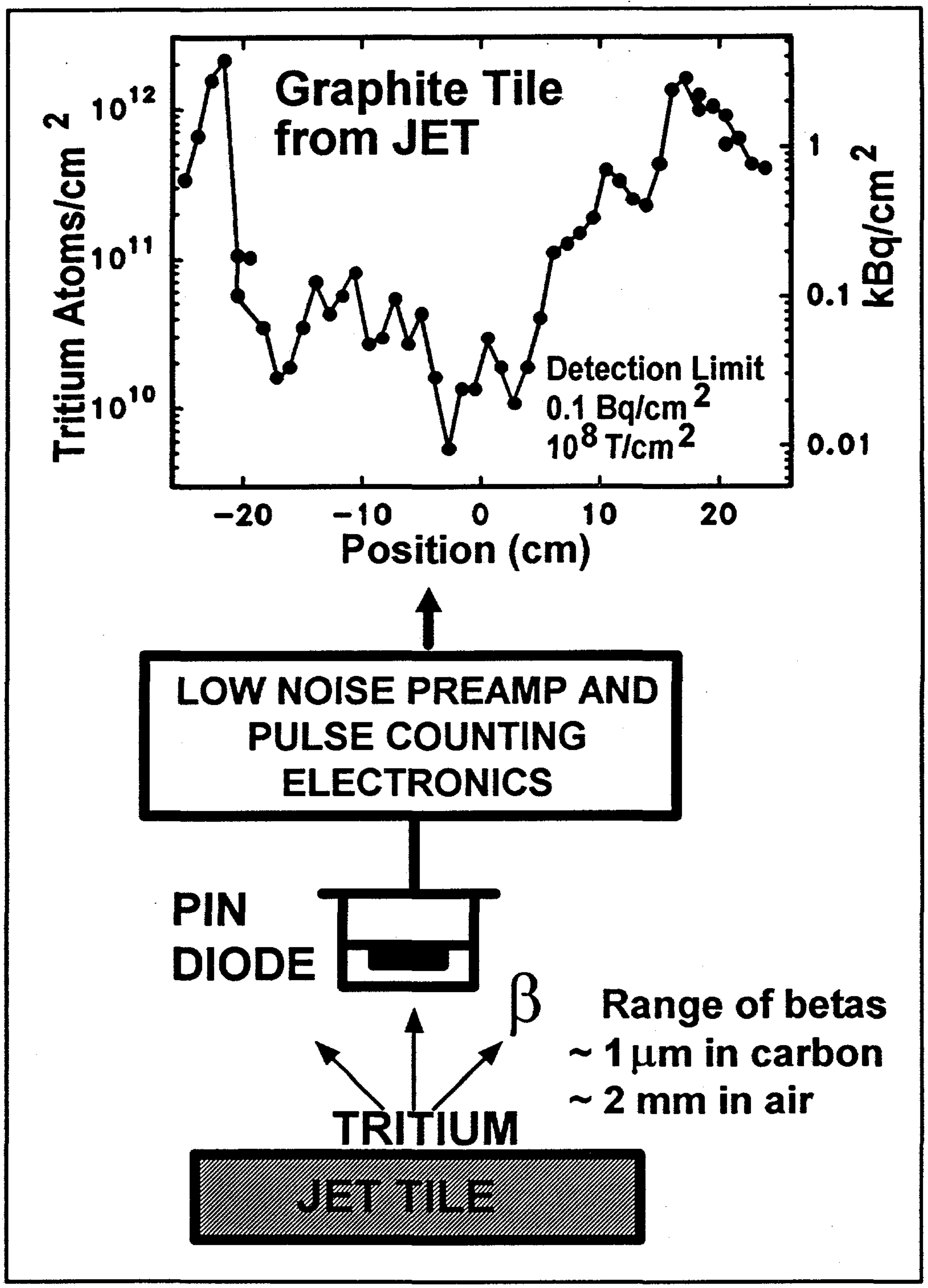
TRITIUM SURFACE CONTAMINATION MONITOR



LOW NOISE PREAMP AND PULSE COUNTING ELECTRONICS

PIN DIODE

Range of betas
~ 1 µm in carbon
~ 2 mm in air

Counting betas using a PIN diode in air or vacuum provides quick real-time nondestructive measurement of tritium near surfaces.

Theory of Atoms Bonded Near Surface Steps Identifies Preferred Bonding Geometries

by P. J. Feibelman and J. S. Nelson

Motivation — The behavior of atoms near surface steps plays a key role in crystal growth and in preparation of materials that are artificially structured on a nanoscale and in surface chemical reactions, e.g., catalytic processes and CVD. To improve control of such phenomena, we wish to know what determines where and how strongly atoms bind to and what governs atom motion near steps. Ordered, stepped surfaces are an excellent laboratory for studying atom-step interactions. They can be well-characterized experimentally. Their periodicity reduces the computational challenge they pose. We have developed computer codes that permit study of perfectly ordered, stepped surfaces, and a unique computer program allowing analysis of isolated impurity atoms bonded to otherwise perfect crystalline surfaces. Thus, we are well-positioned to advance the understanding of atoms near surface steps.

Accomplishment — We carried out the first calculation from first-principles of the atomic arrangement of a stepped surface. The results, for Al(331), are in remarkable agreement with an experimental, Low Energy Electron Diffraction (LEED) study. We computed the energy versus position for H, S, and Al atoms bound to Al(331) as a function of their locations on the surface, finding that both the optimal binding sites and the minimum barriers to motion are different for the three species of atom. An extra Al on the stepped surface prefers to bind in the 5-fold coordinated, epitaxial growth site at a step bottom while H and S atoms prefer 1- and 2-fold coordination sites, respectively, on step edges where they can simultaneously satisfy their valence requirements and passivate the least well-coordinated surface atoms. H atoms can easily migrate along step edges while S atoms can freely "wag" about an edge. The unexpected variety of binding sites and motional preferences confirms the need for further studies aimed at controlling kinetics and growth.

Significance — This work affects the interpretation of surface structural experiments. We confirmed a LEED analysis for a complex surface and provided a physical explanation for the unusual pattern of atomic positions that was found. Our results promise to help interpret data from the novel, Scanning Tunneling and Atomic Force Microscopies, which allow us to see atoms adsorbed near steps. Our conclusions concerning preferred binding arrangements and barrier geometries will affect the description of kinetics on stepped surfaces - whether atoms compete for similar sites and whether atoms block each others' motion, or not, will significantly affect reactivity and diffusion rates.

Keywords: surface defects, surface impurities, electronic and geometric structure of surfaces

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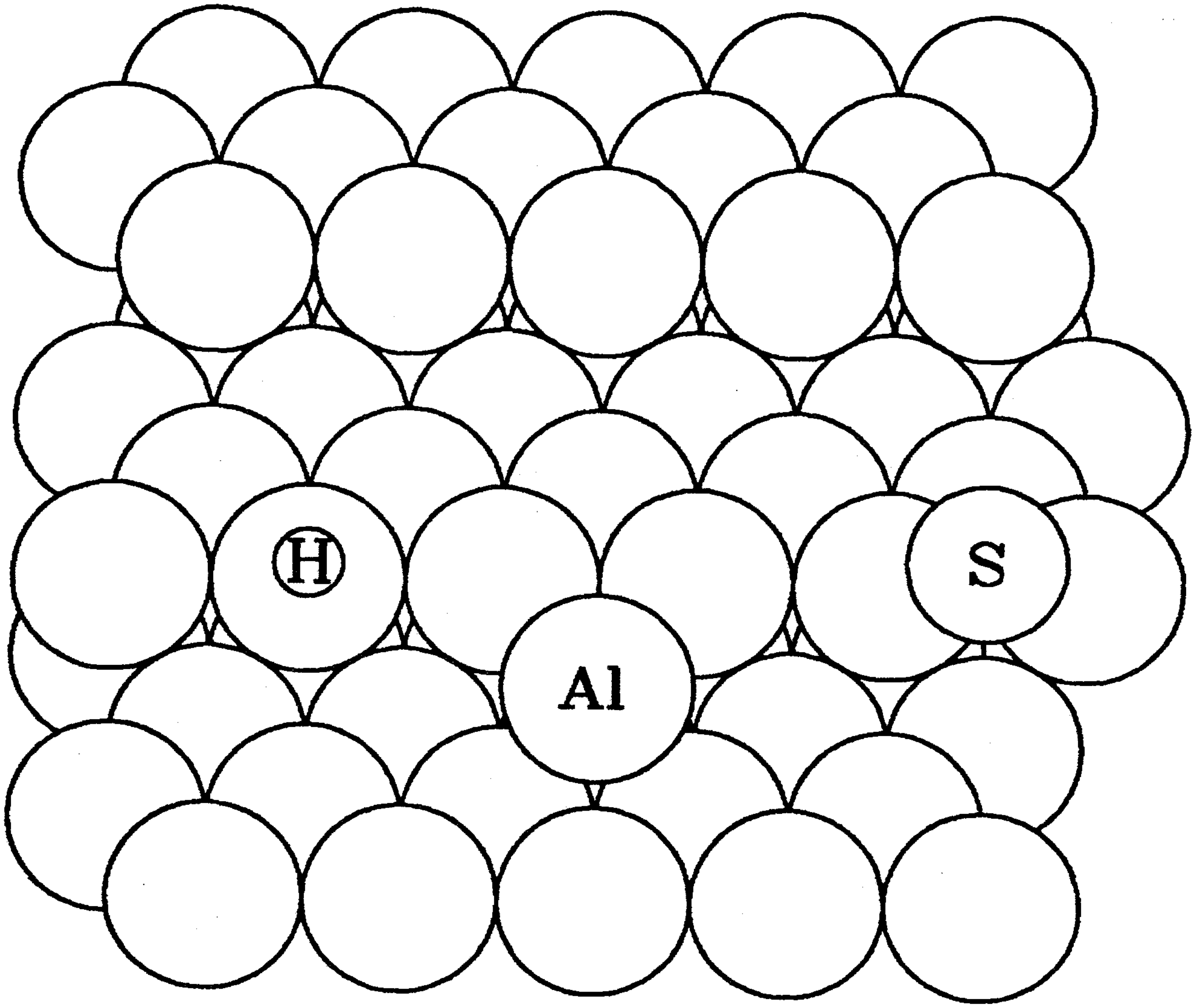

Schematic of Al(331) surface showing favored locations of adsorbed atoms.

Electric Fields Control Atom Motion on Surfaces

by **G. L. Kellogg**

Motivation — The fabrication of artificially structured materials with unique and tailorable properties (electrical, optical, structural, magnetic, etc.) requires both an atomic-level understanding of how crystalline films grow and the ability to control the fundamental steps in the growth process. It is widely recognized that the diffusion of individual atoms on surfaces plays a key role in the growth of crystalline solids and epitaxial thin films. In past investigations we have shown that the migration of atoms may proceed by a mechanism involving exchange between the diffusing atom and an atom within the surface layer. This new type of surface diffusion has attracted considerable recent attention, both as an alternative mechanism for atom transport across surfaces and a new means for surface alloying during thin film growth.

Accomplishment — We have discovered that one can control the rate of exchange-type displacements with an externally applied electric field. A positive field (sample biased positively) decreases and a negative electric field increases the diffusion rate. The surprisingly large magnitude of the effect is illustrated in the accompanying figure which shows the field dependence of the measured activation energy of surface diffusion (the energy barrier to individual displacements) for Pt atoms on Pt(100). As indicated schematically on the figure, inhibition of exchange displacements causes the energetically favorable diffusion mode to change from exchange to hopping at higher fields. Thus, one can select the mode by which atoms move on a surface with an externally applied electric field. The field effect is explained by an electron-transfer process which changes the bonding of the diffusing atom to neighboring surface atoms. This interpretation is beginning to provide some insight as to why exchange displacements are favored in some systems and hopping in others.

Significance — The ability to change both the diffusion rate and the transport mechanism for atoms on surfaces means that it should be possible to control the growth mode of crystalline materials with an externally applied field. In heteroepitaxial systems, electric fields could also be used to prevent unwanted interdiffusion effects due to the exchange mechanism. Understanding and controlling the growth modes of crystalline solids is one of the major goals in our Basic Energy Sciences/Material Science program on Tailored Surfaces and Interfaces for Materials Applications. These results also point to the importance of external electric fields in attempts to study surface diffusion and manipulate individual atoms by scanning probe microscopies where comparable electric fields are present.

Keywords: advanced materials, artificially structured materials, crystal growth, thin film growth, surface diffusion, surface alloying, atomic exchange, electric fields, field ion microscopy

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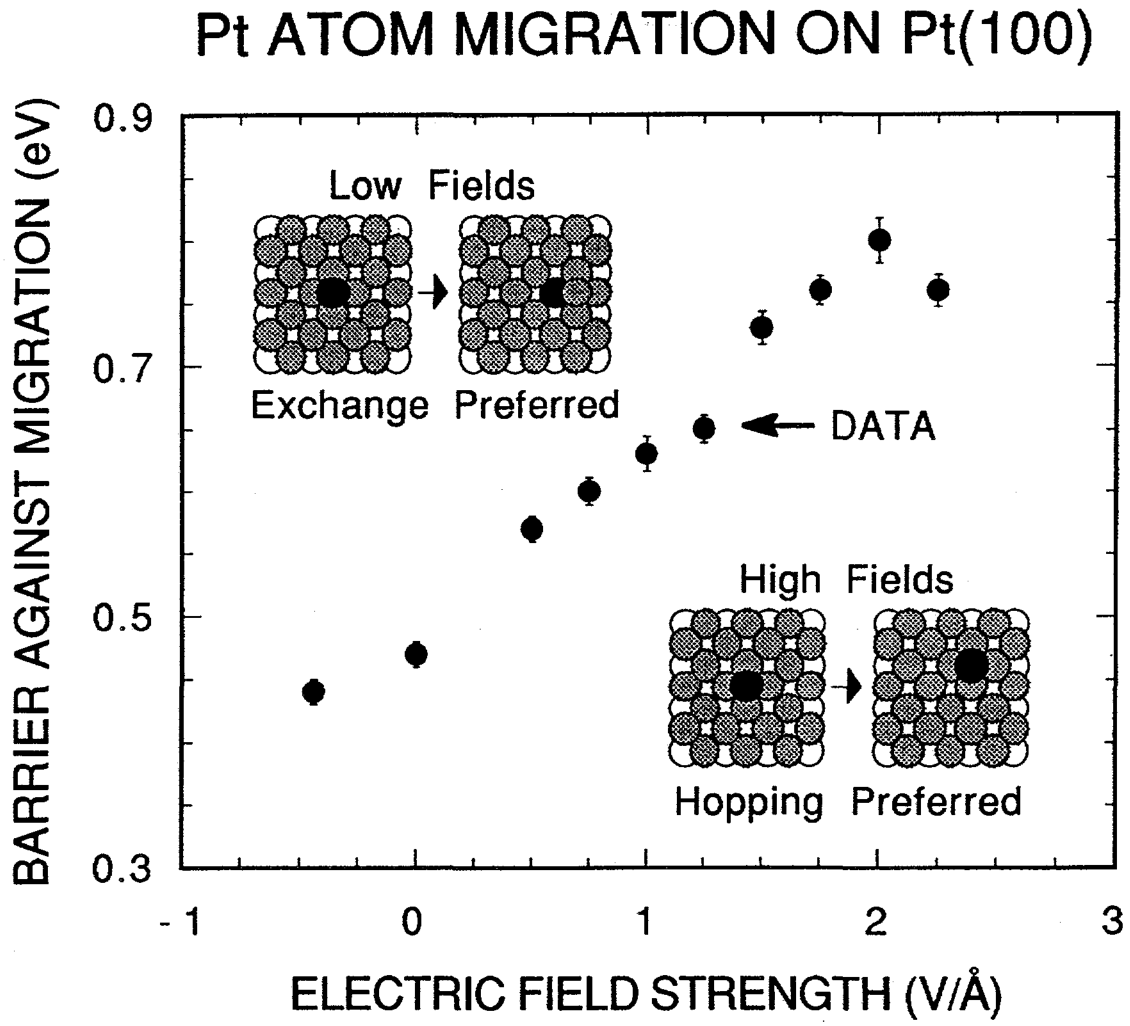

Pt ATOM MIGRATION ON Pt(100)

The activation barrier for diffusion of Pt atoms on the (100) surface of Pt decreases when a negative electric field is applied and increases when a positive electric field is applied. At electric field strengths above 1.5 V/Å, the energetically favorable diffusion mode changes from exchange-type displacements to hopping-type displacements.

High-Pressure, Shock-Compression Studies of Porous Materials Identify Basic Complexities of the Processes

by **R. A. Graham**

Motivation: Issues of materials synthesis and processing under shock-compression as well as safety of high explosives in industrial and military applications revolve around deformation and chemical processes in shock-compressed, porous powders. Resolution of underlying technical issues rests upon detailed experiments on responses of porous powders in both single-component and multiple-component configurations. There is little information in kinetics of deformation processes as revealed in stress pulse "rise time" observations or on pressure required to compress a porous materials to full density.

Accomplishment: Experimental capabilities for time-resolved pressure measurements with PVDF piezoelectric polymer stress gauges have been improved so that recording times of several microseconds are routinely achieved. With this capability in hand, we have completed a series of experiments on a single-component, porous powder compact, TiO_2, a two-component compact, $2Al+Fe_2O_3$, a chemically reacting, two-component system, 5Ti+3Si, and a porous high explosive HMX. Typical experimental observations are shown in Figure 1 which shows a schematic of the experimental arrangements along with typical experimental records and the resulting pressure-versus-time observations for a porous HMX explosive which reacts chemically as a result of the loading. Piezoelectric current-versus-time measurements provide a direct measure of rate of change of stress in time. Upon integrations of the current pulses, stress-versus-time data are obtained. Considerable detail on the compression process is revealed. The rise time data of Figure 2 shows explicit kinetic data on the deformation process. At low pressure, when the compression is incomplete, the rise times become extraordinarily long. The stress-volume response of two powders, single component TiO_2, and two-component 5Ti+3Si are shown in Figure 3. Not shown are the compression data on a $2Al+Fe_2O_3$ mixture which show an unusually complex compression process.

Significance: The measurements on shock compression of porous powders show that the processes are much more complex than our current ability to model them. Thus, the work provides the basis for a new generation of modeling to realistically describe such events.

Keywords: high pressure, shock compression, porous powders, porous high explosives, stress pulse measurements, stress pulse rise time, pressure-volume relationships

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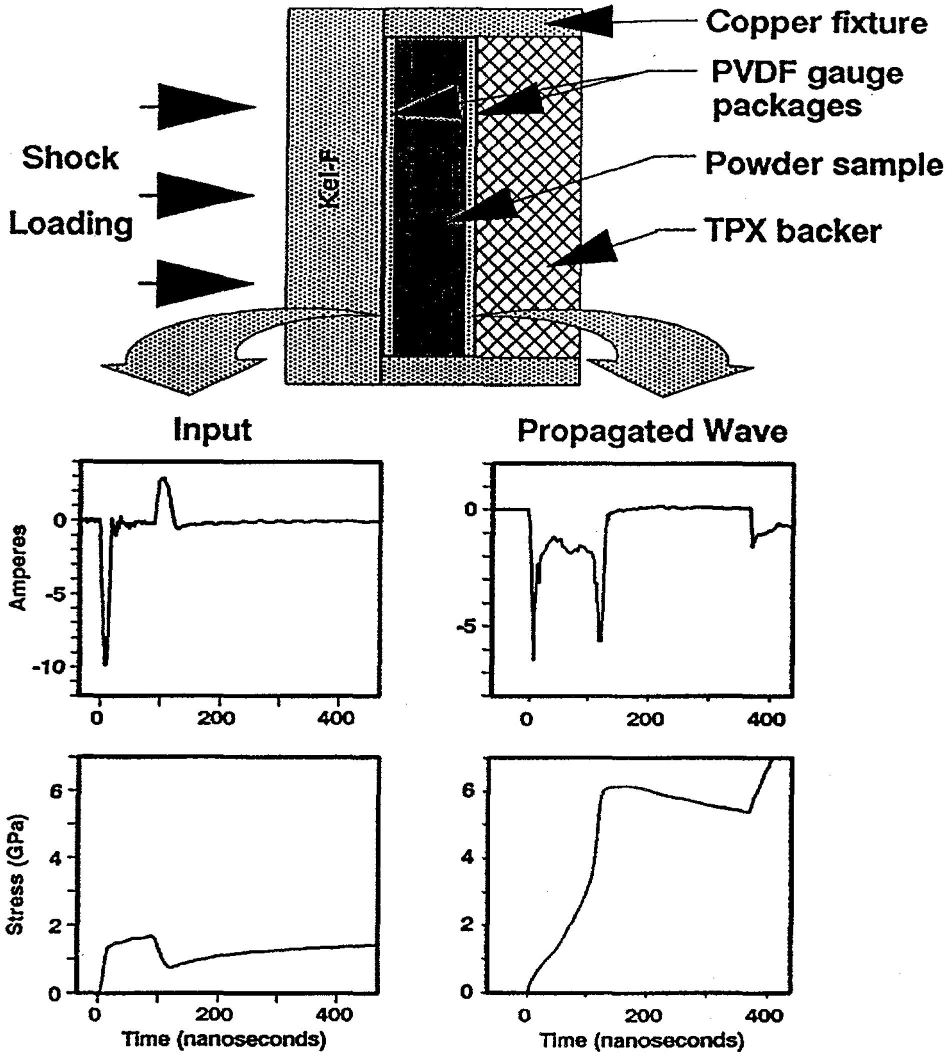

Figure 1. The experimental arrangement and typical records for measurement of shock response of powders.

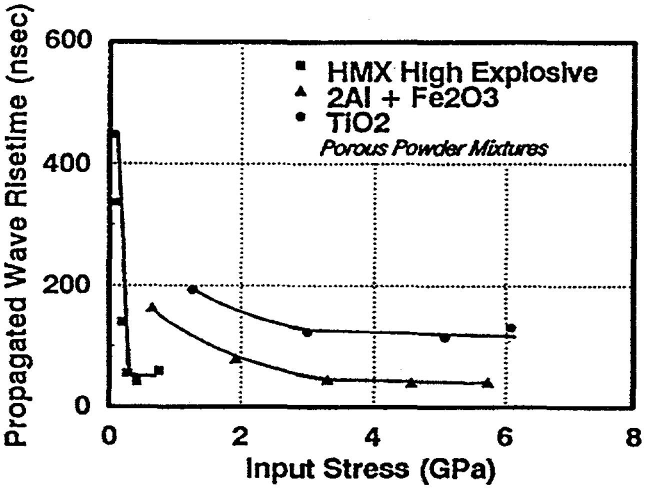

Figure 2. Observed rise times of propagated stress pulses as shown provide direct data on deformation kinetics.

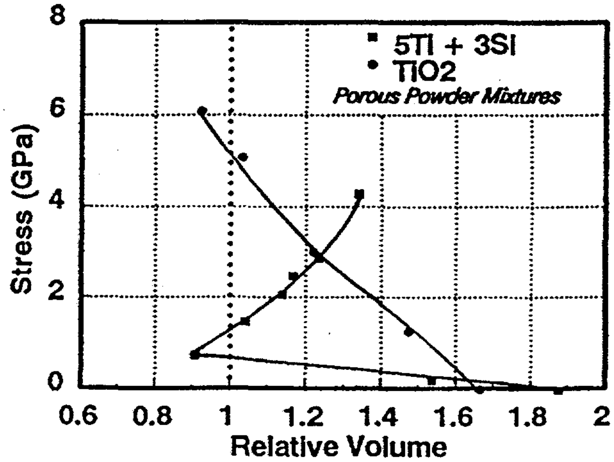

Figure 3. Stress-volume data reveal stress to deform powders to solid density and any resulting chemical reaction. The Ti/Si powders show strong chemical reaction.

Evolution of Structure in an Electroheological Fluid Identifies Microscopic Time-Dependent Processes of Solidification and Strength

by **J. E. Martin**

Motivation — Electroheological (ER) fluids are particle dispersions that reversibly solidify in the presence of an electric field. The rapid solidification response, which occurs in a few milliseconds, makes ER fluids ideal for fast electromechanical applications, such as automotive and robotic clutches, shock absorbers, etc. However, the mechanism of solidification, including the structural changes that occur after the field is applied, is not well understood. Qualitative microscopy studies show that when an electric field is applied to an ER fluid, the polarized particles first chain along the field lines, the chains then aggregate to form columns, and the columns aggregate to form thicker columns *ad infinitum.* The kinetics of this process holds important clues to the remarkably subtle forces that cause column formation.

Accomplishment — We have constructed a real-time light scattering apparatus with a two dimensional CCD array as a detector that enables us to study the evolution of structure in a nearly index matched colloidal silica ER fluid as a function of applied voltage and particle concentration. We have found that when an electric field is applied to the quiescent fluid, spheres form chains along the electric field lines and cause strong light scattering lobes to appear at a finite scattering wavevector q orthogonal to the field lines (see figure). These lobes then brighten as they move to $q=0$, indicating the existence of an unstable concentration fluctuation that signifies the segregation of chains into columns. In fact, the observed power law growth kinetics of the column width ($\propto t^{2/5}$ in figure) as well as the form of the structure factor, are *qualitatively* similar to two-dimensional spinodal decomposition in a system with a conserved order parameter. When the sample is subjected to shear, we find that the scattering pattern approaches a steady state, with lobes that are rotated in the direction of fluid vorticity. The angle of rotation is found to increase as the cube root of the shear rate, in agreement with our theoretical prediction of the steady state structure of fragmenting particle chains.

Significance — We were surprised to find that although solidification of an ER fluid occurs in milliseconds, column formation occurs on a time scale of minutes. This disparity in time scales occurs because although the dipolar forces that cause particles to chain and the macroscopic fluid to solidify are large, the interaction between chains is very weak due to the cancellation of interactions by image dipoles in the electrodes. In fact, the only remaining source of interaction between chains is through the weak coupling of their fluctuations in dipole density. A particular consequence of this is that although solidification occurs rapidly, the strength of an ER fluid will continue to increase for several minutes.

Keywords: electrorheological fluids, light scattering, colloids, mode-mode coupling

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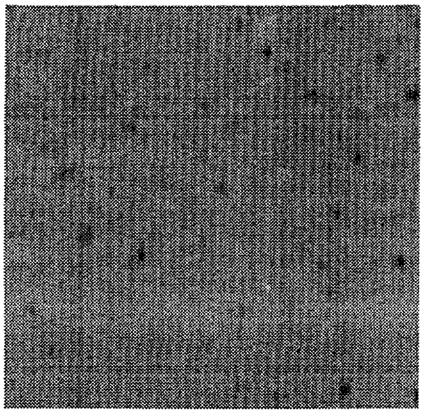
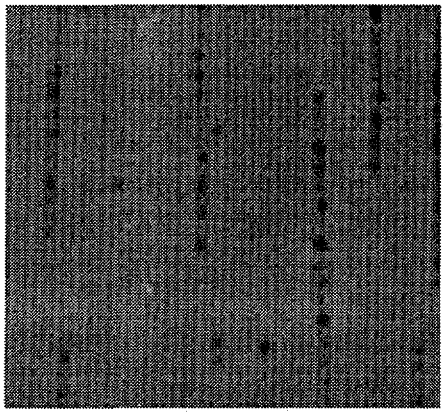
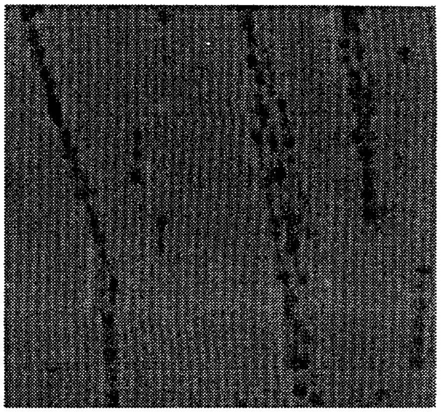
Evolution of Structure in an ER Fluid



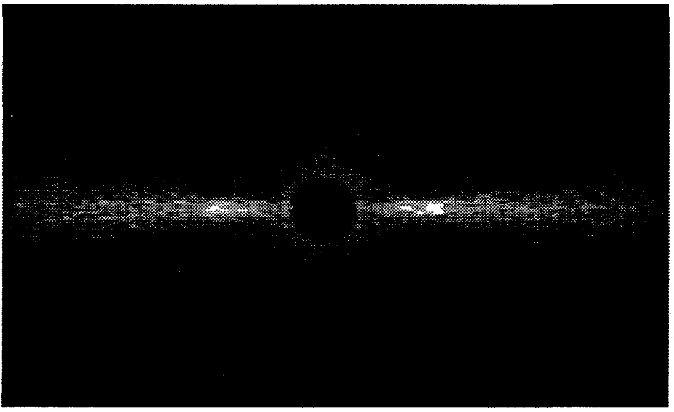
spheres



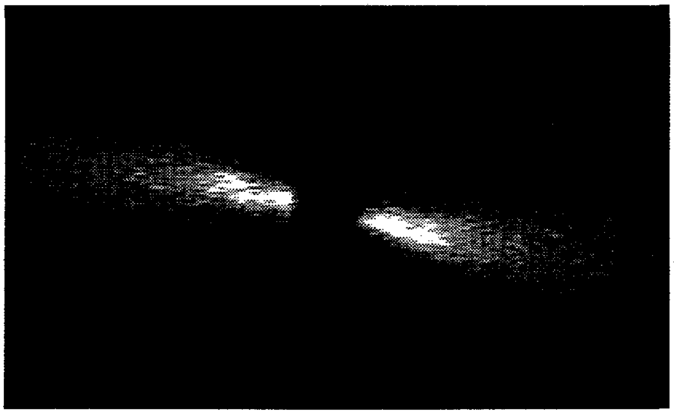
chains



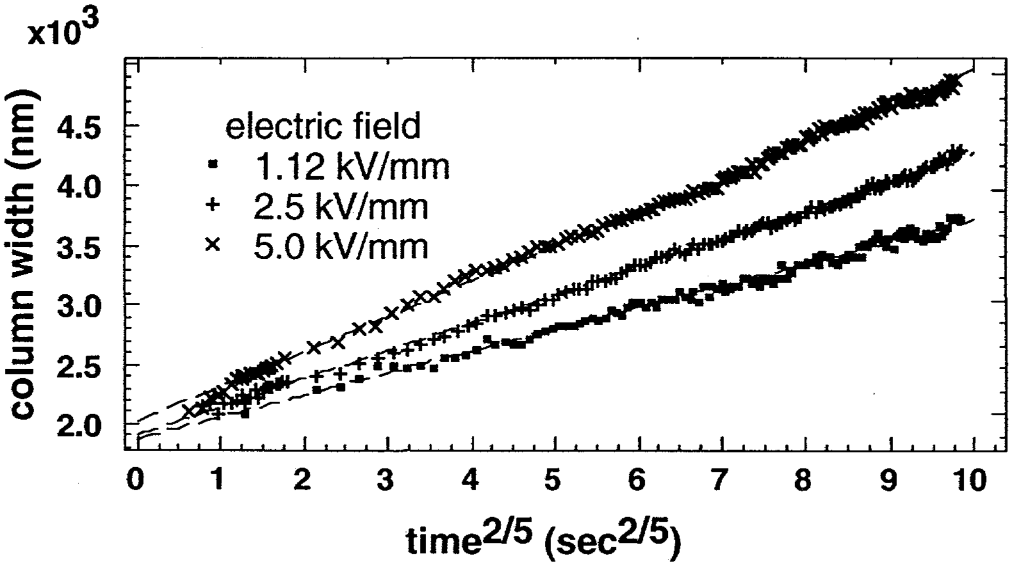
columns



scattering from quiescent fluid



... sheared fluid



- *The column width increases as a power of time.*

Interface Strain in Lattice Matched III-V Semiconductor Superlattices can be Calculated and used to Modify Semiconductor Superlattices

by **J. S. Nelson, S. R. Kurtz, L. R. Dawson, and J. A. Lott**

Motivation — The ability to optimize the electronic and optical properties of semiconductor devices through interface engineering opens up a new realm of band gap technology. It is well known that strain within the layers of lattice-mismatched semiconductor superlattice can be used to improve device performance; it is less well known that interface layering and alloying can have a similar effect. In this work we demonstrate the fundamental role played by intrinsic interface strain in determining valence and conduction band offsets in lattice-matched semiconductor superlattices. In these systems, when both the group III and V sublattices are different, large strains can develop at the interface with little or no strain in the layers (top figure). These strains can be relieved by localized tetragonal distortions at the interface, resulting in changes in the local interface dipole. Since band offsets are very sensitive to the interface electrostatics, interface strain can have a significant effect on the optical and transport properties of III-V semiconductor superlattices.

Accomplishment — Combining first-principles theoretical energy band structure methods with experimental infrared photoluminescence spectroscopy, we have determined the effects of intrinsic interface strain on the electronic and optical properties of lattice matched $Al_{0.8}Ga_{0.2}As_{0.14}Sb_{0.86}$/InAs. The predicted energy levels for a 100Å $Al_{0.8}Ga_{0.2}As_{0.14}Sb_{0.86}$/InAs superlattice are compared to infrared photoluminescence measurements in the bottom figures. Including the interface strain effects, the calculations predict a type II band alignment with a lowest excitation energy of 0.29 eV (valence band offset of 0.24 eV), in excellent agreement with the experimental value of 0.32 eV. If the interface strain is neglected in the calculation, the valence band offset is only 0.05 eV. This result demonstrates the sensitivity of the electronic and optical properties of semiconductor superlattices to interface specific modifications (in this case interface strain).

Significance — This research has led to a more complete understanding of the role of interface specific effects and their influence on electronic and optical properties of semiconductor superlattices. These fundamental results offer the possibility of modifying the properties of semiconductor superlattices through interface engineering.

Keywords: microelectronics and photonics, semiconductor interfaces, semiconductor superlattices, InAs, AlGaAsSb, band structure

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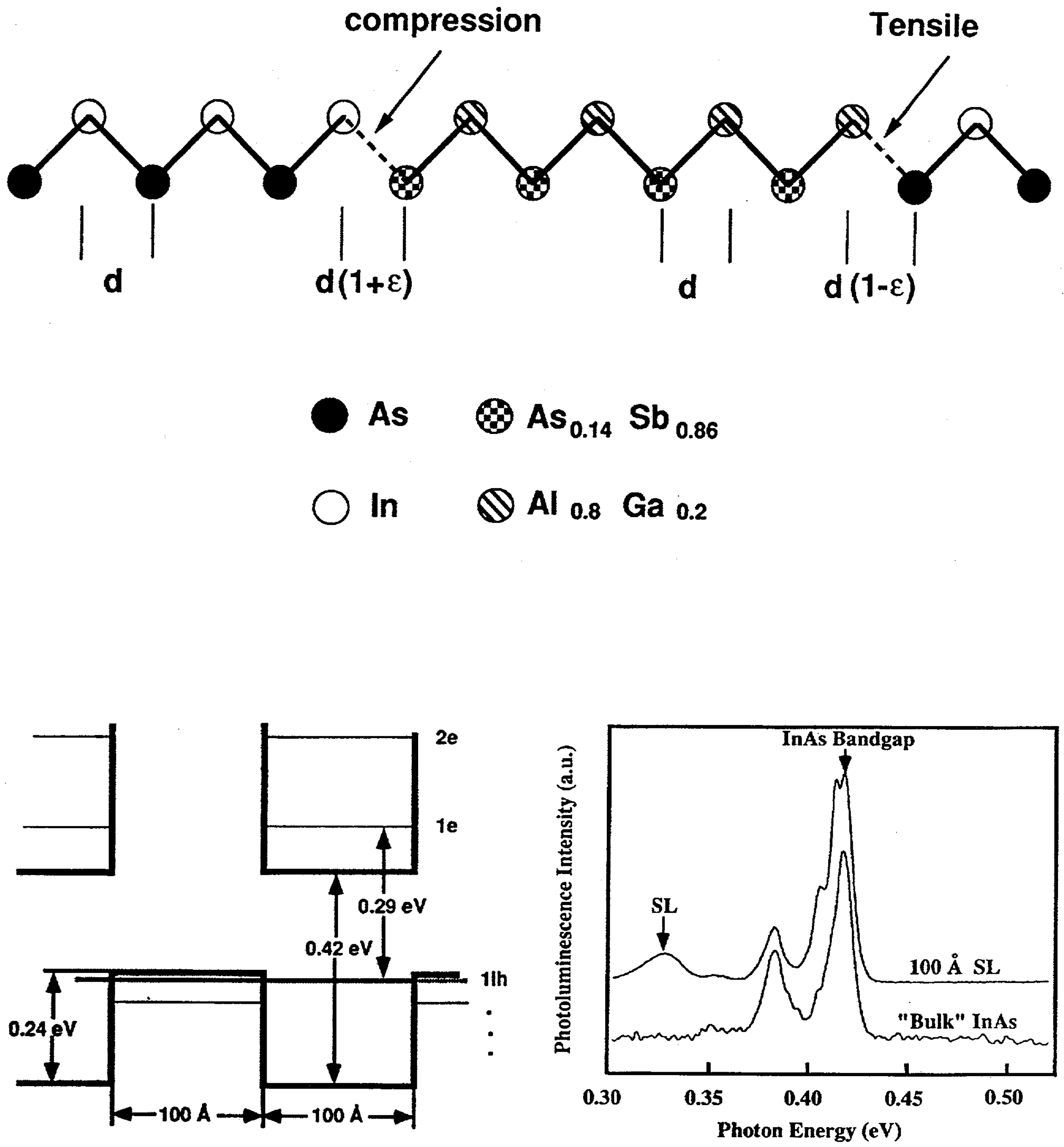

Schematic illustration of the InAs/$Al_{0.8}Ga_{0.2}As_{0.14}Sb_{0.86}$ interface (upper figure). The In-$As_{0.14}Sb_{0.86}$ and $Al_{0.8}Ga_{0.2}$-As bonds are under nearly equal and opposite compressive and tensile strains, respectively. The predicted band offsets and energy levels are given in the lower left figure. A lowest excitation energy of 0.29eV is in good agreement with a value of 0.32eV obtained from Infrared photoluminescence measurements (lower right).

Phosphorus Doping of Boron Carbide Semiconductors Improves Feasibility of n-Type Doping

by **T. L. Aselage and D. Emin**

Motivation — Crystalline solids containing boron and carbon in ratios between 10 to 1 and 4 to 1 are called boron carbides. These solids have very high melting temperatures, greater than 2400° C. Our prior research has shown that boron carbides are p-type semiconductors, in which the charge carriers that contribute to electrical conduction are positively charged "holes". Semiconducting boron carbides may be useful as very efficient, high-temperature thermoelectric materials. Thermoelectric power generation utilizes a difference in temperature between the ends of a semiconducting material to generate a voltage. To complete the electrical circuit and use this thermoelectric voltage to do work, an n-type semiconductor, in which current is carried by negatively charged electrons, is required to complement the p-type semiconductor. We are attempting to produce an n-type boron carbide for compatibility with our efficient p-type boron carbides.

Accomplishment — One approach to producing an n-type boron carbide is to substitute an electron donor such as phosphorus for boron or carbon. We have prepared homogeneous samples with a phosphorus atom incorporated into up to ten percent of boron carbide's 15-atom unit cells. Raman spectroscopy and x-ray diffraction show that P-B or P-C groups replace some of the C-B-C chains present in undoped boron carbide. We have previously associated the two modes centered about 500 cm^{-1} in the Raman spectra shown in the accompanying figure with vibrations of the C-B-C chains. The intensities of these modes decrease with increasing phosphorus doping consistent with phosphorus substitution at this chain site. Although the $x = 0.2$ and 0.35 samples were multi-phase, the decreasing intensity in the 500 cm^{-1} bands of these samples suggests that the phosphorus content in boron carbides can be increased beyond that achieved in homogeneous samples ($x = 0.10$). While our measurements of the thermoelectric power show that the homogeneously doped samples are still p-type, their electrical conductivities are significantly lower than undoped boron carbides as shown in the accompanying figure. Our analysis of the data suggests that the hole concentration in these doped samples is reduced by as much as 70% relative to undoped boron carbides. A small additional increase in dopant concentration (to $x > 0.15$) should lead to n-type material.

Significance — Thermoelectric power generation is useful in situations that require high reliability, such as power generation in space. Boron carbide elements could enhance conversion efficiency by increasing both the figure-of-merit of the semiconductor and the maximum operating temperature. Illustration of the feasibility of doping with phosphorus is a significant step toward producing an n-type boron carbide and the construction of an all-boron carbide thermoelement. More generally, the introduction of phosphorus into boron carbides has provided confirmation of our ideas regarding the structure and electrical properties of boron carbides.

Keywords: advanced materials, boron-rich solids, thermoelectrics

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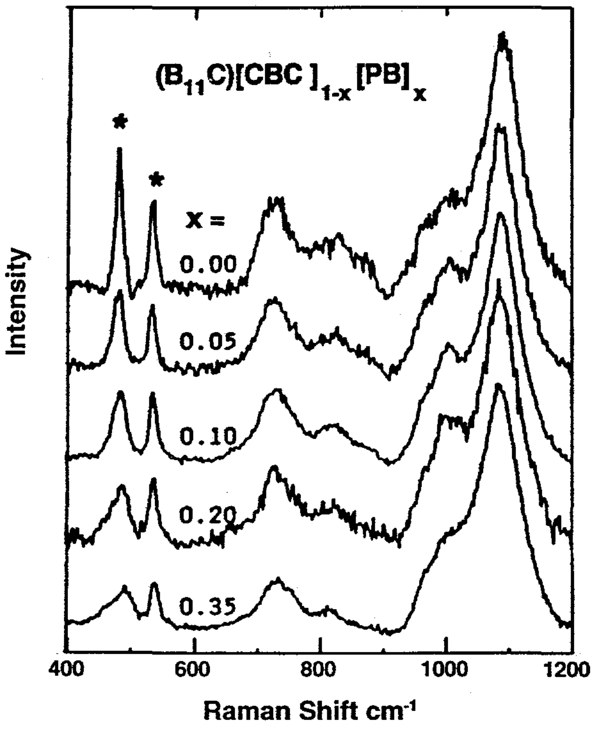
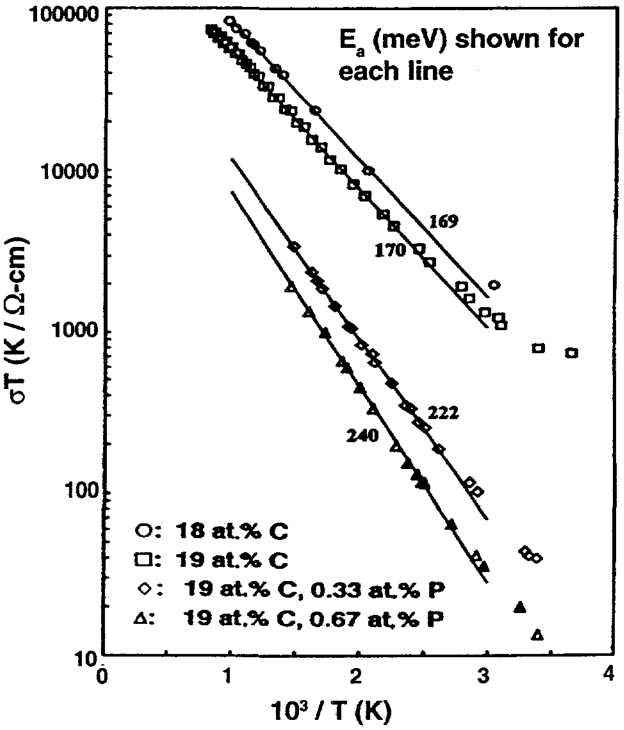
Phosphorus Doping of Boron Carbide



Decrease in intensity of indicated Raman bands suggests a chain location for P atoms.



DC conductivity is reduced by lowering the carrier density and increasing the activation energy.

Novel Nanocluster Materials have been Developed for Energy Applications and Show Significantly Improved Catalytic Activity

by **J. P. Wilcoxon**

Motivation—The development of technologies that enable the efficient use of energy resources is critical for the security and economic well-being of the U.S. Since coal reserves in the U.S. are the largest potential source of hydrocarbon fuels, an economically viable method to liquify coal would have enormous impact. Nanoclusters are extremely reactive materials due to their enormous surface/volume ratio and the abundance of non-classical surface sites. This greatly enhanced surface activity may allow inexpensive materials, such as iron and iron sulfide, to be used as catalysts since the catalytic properties of nanoclusters can be tuned by varying cluster size. Also, the optical, electronic, and magnetic properties of clusters can be tuned by varying cluster size. This variability is important for other potential applications which include photocatalysis, information storage, non-linear optics, optical detectors, electronic switches, and capacitors. However, a principal barrier retarding the utilization of nanoclusters is the lack of appropriate synthesis techniques.

Accomplishment—We have developed and patented a unique nanocluster synthesis method that uses inverse micelles as reaction vessels. This process leads to a wide range of nanocluster materials, including metals, metal alloys, semiconductors, and metal sulfides and oxides. Since this is a wet chemical technique using inexpensive starting materials, the process can be economically scaled to produce large quantities. In collaboration with Sandia's fuel sciences programs sponsored by DOE/PETC, we have demonstrated excellent catalytic activity for coal liquefaction using novel nanocluster materials such as iron and iron sulfide which are not conventional catalysts in bulk form. The figure shows the greatly increased catalytic activity of palladium clusters with decreasing cluster size for pyrene hydrogenation, a model reaction for coal liquefaction. We have also synthesized several new nanosize semiconductor materials such as MoS_2 and FeS_2 whose bandgap can be adjusted by changing the cluster size. We have investigated the optical, magnetic, and dielectric properties of metal nanoclusters.

Significance — Our nanosize clusters are the only inexpensive iron materials to exhibit significant catalytic activity in coal liquefaction processes. This may allow disposable catalysts to be developed which can provide a new source of hydrocarbon fuels via coal liquefaction. The ability to synthesize semiconductor nanoclusters with tailorable band-gaps can replace conventional powders of TiO_2 in solar applications ranging from photocatalytic fuel production to solar detoxification. Presently available materials have the wrong bandgap for these applications, while nanosize MoS_2 and FeS_2 can be precisely tailored to match the solar spectrum.

Keywords: advanced materials, process science, nanocluster synthesis, coal liquefaction, photocatalysis, solar detoxification

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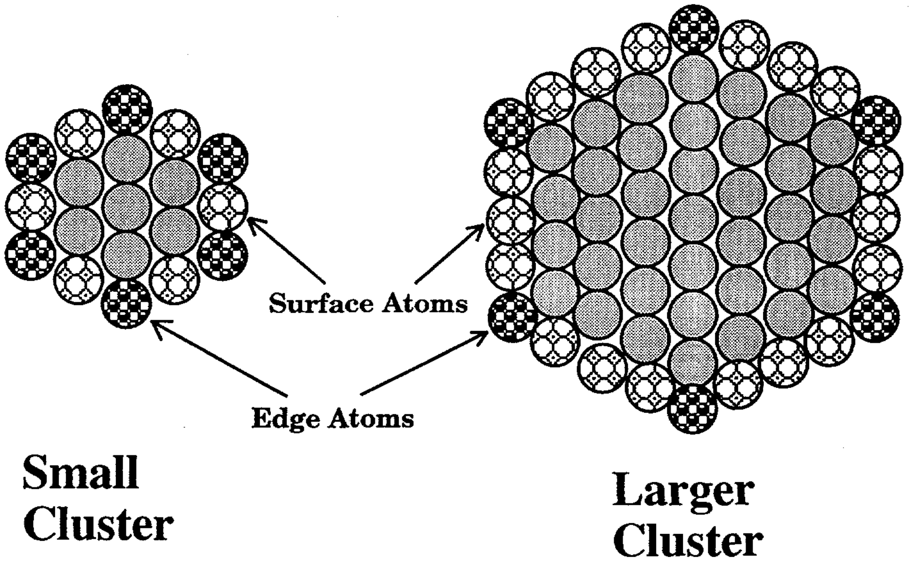
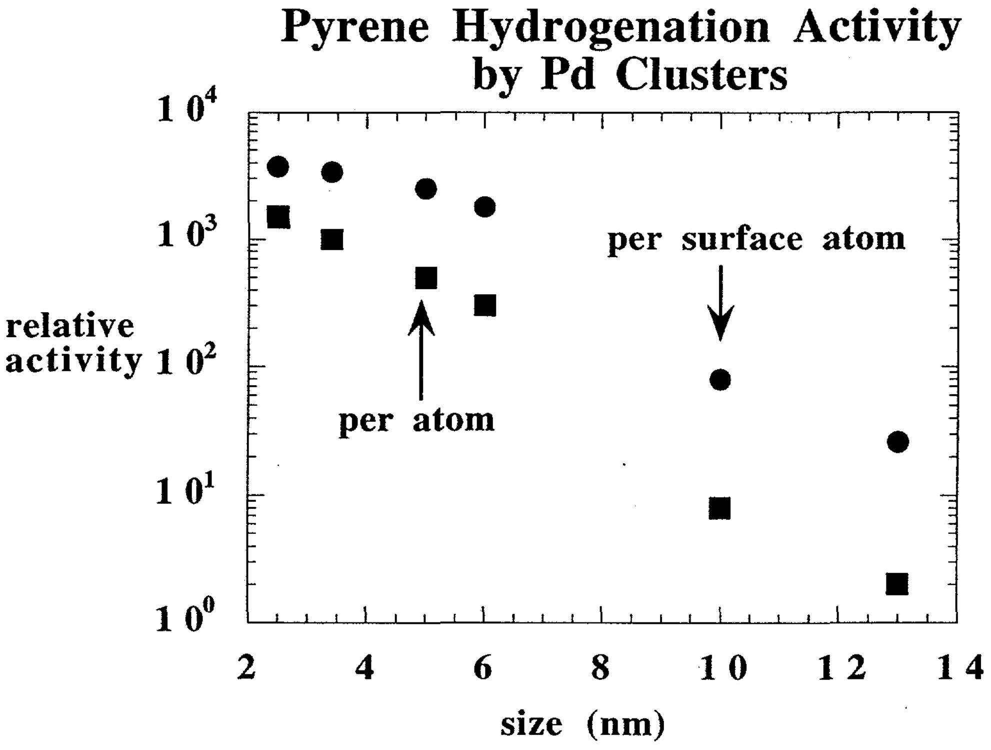
Nanoclusters for Energy Applications





As indicated above, small clusters have a higher ratio of surface and edge atoms to total atoms than do large clusters. In addition, the enhanced catalytic activity of smaller clusters per surface atom may be due to their more highly faceted, defective surfaces

Gettering of Copper Impurities by Nanocavities in Silicon is Greatly Superior to that by Silicide Precipitation

by S. M. Myers and D. M. Follstaedt

Motivation — Metallic impurities degrade the performance of silicon-based microelectronics, even at extremely low impurity concentrations that extend below the sensitivity of analytical probes. For this reason, clean-room processing is often supplemented by "gettering", a process in which impurity traps are introduced into non-critical regions of the device. At present, these traps consist of defects in the silicon which serve as nucleation sites for precipitation of metal impurities as metal-silicide compounds. A more potent gettering method is needed which will reduce the concentrations of mobile impurities to still lower levels and which is capable, unlike present methods, of actually dissolving unwanted metal-silicide precipitates from critical regions of devices. Here we report BES/MS supported research showing that copper, a representative detrimental impurity, is strongly gettered by nanometer-size cavities formed in silicon by helium ion implantation. Sandia is uniquely positioned to conduct this research because of its extensive expertise and facilities in the areas of microelectronics and ion-beam modification of materials.

Accomplishment — We demonstrated that ion implantation of helium into silicon at an energy of 30 keV and a dose of 200 ions/nm^2 or greater forms a high density of nanometer-size cavities that remains stable at least to 1100° C, thereby covering the temperature range of standard microelectronics processing. The cavities are shown in the accompanying cross-section transmission-electron micrograph. Rutherford backscattering analysis after heating of the material indicated that copper impurity atoms are trapped at the cavities with a binding energy of 2.2 eV per atom. By comparison, the binding of copper in the silicide precipitates presently used for gettering is only 1.6 eV per atom. The greater strength of cavity gettering was further demonstrated by observing that cavity traps on one side of a wafer can actually dissolve copper-silicide precipitates on the opposite side. This strong trapping is ascribed to the chemical reaction between copper atoms and unsatisfied silicon bonds on the walls of the cavities.

Significance — Cavity gettering of copper impurities in silicon provides three potential advantages over the presently used gettering by silicide precipitation: 1) orders-of-magnitude greater reduction of the copper concentration in solution in silicon, 2) dissolution of unwanted copper-silicide precipitates in critical areas, and 3) compatibility of the process with gettering from the front, device side of wafers as well as from the back side. Cavities may provide similarly superior gettering of other metallic impurities, an issue to be addressed by further research.

Keywords: microelectronics, process science, silicon, metal impurities, gettering

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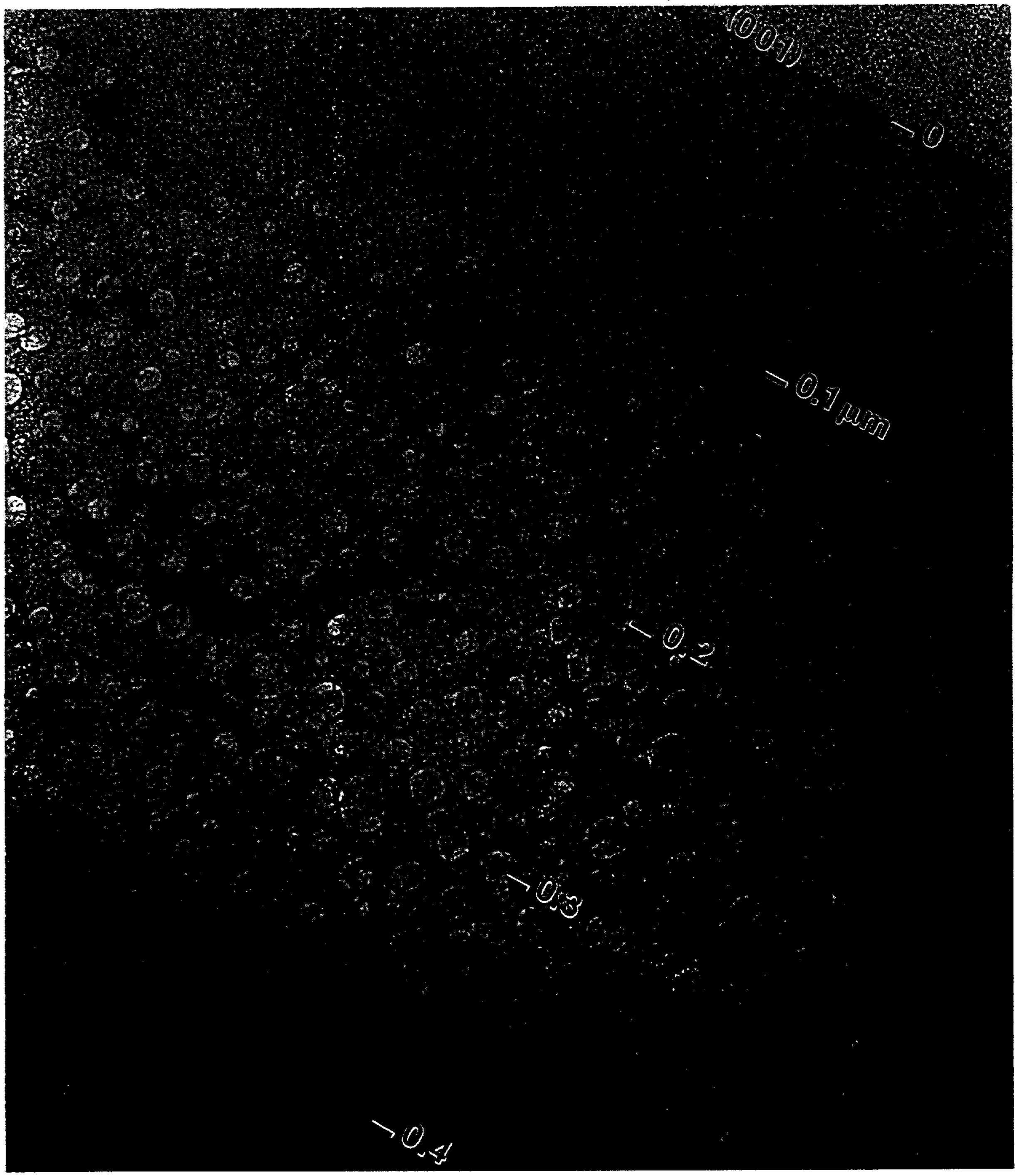
CAVITIES IN He-IMPLANTED Si



[110] Cross Section TEM

1x10^{17} He/cm^2, 30 keV; 1/2 hr. at 700°C

High Pressure Results Support the Identification of EL2 as the Arsenic Antisite Defect in GaAs

by **G. A. Samara**

Motivation — It is well recognized that crystalline imperfections and impurities produced during growth or device processing can introduce deep energy levels into the bandgaps of semiconductors. These levels act as carrier trapping, recombination and scattering centers, and thus have a strong influence on electronic properties and device performance. The increasing technological importance of the group III-V semiconductors, especially GaAs, is focusing attention on the need to understand and control their defect properties. Unfortunately, at present very little is known about defects in these materials. To be specific, while a large number of deep levels have been observed in GaAs, in almost all cases the responsible defects remain unknown because of the lack of suitable microscopic probes for identifying them. In earlier work we showed that pressure is a very useful variable in the study of defects and deep levels providing insights into the physics, nature of deep level potentials, and breathing mode lattice relaxations accompanying the formation of defects as well as carrier emission and capture processes by deep levels. Pressure results often make it possible to test proposed models, and in conjunction with theory, allow identification of the microscopic defects responsible for the deep levels. These considerations motivated our study of EL2, the dominant defect in melt-grown and vapor-phase epitaxially grown GaAs. Technologically EL2 controls the electronic properties of semi-insulating GaAs by pinning the Fermis level and scientifically its microstructure remains not fully established despite extensive research.

Accomplishment — EL2 produces two in-gap deep levels: the first donor (0/+) level located E_c-0.75 eV and the second donor (+/++) level located at E_v+.054 eV observed in n- and p-type GaAs, respectively. We have studied the effects of hydrostatic pressure on the electronic emission and capture properties of these two levels and reached the following conclusions: (1) both levels move higher in the bandgap with pressure; (2) relatively large inward (outward) lattice relaxations accompany electron emission (capture) from (by) these levels; and (3) the magnitudes of these relaxations, namely 3.7 and 6.2A^3/electron, respectively (which translate to 2.0 and 3.3% change in near neighbor distance, or agree quantitatively with theoretically results which identify EL2 as the As antisite defect (see Figure). These results, which emphasize the antibonding character of the electronic orbitals which describe EL2, are consistent with and support this identification.

Significance — Our EL2 results agree both qualitatively and quantitatively with expectations for the As antisite defect and thus provide a compelling argument for this identification and the ultimate resolution of the microstructure of this important defect. Definitive identification of this defect is the first important step toward its control. Our pressure technique is at present the only experimental method for quantitatively determining defect-induced breathing mode lattice relaxations.

Keywords: defects, deep levels, pressure, EL2, arsenic antisite, GaAs

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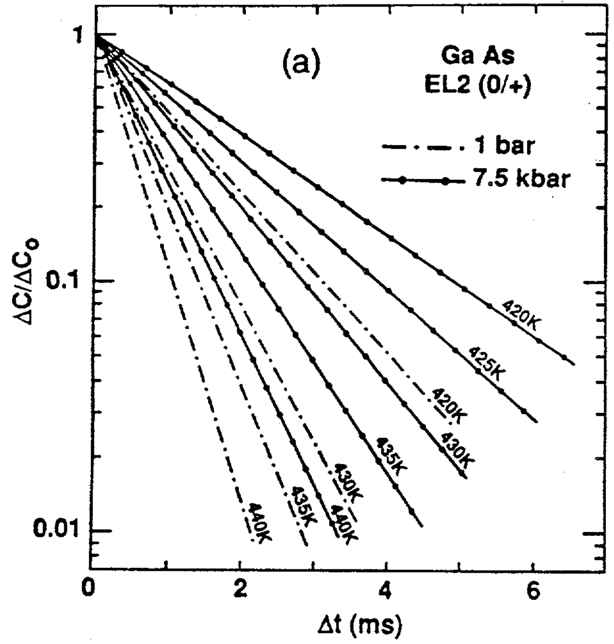
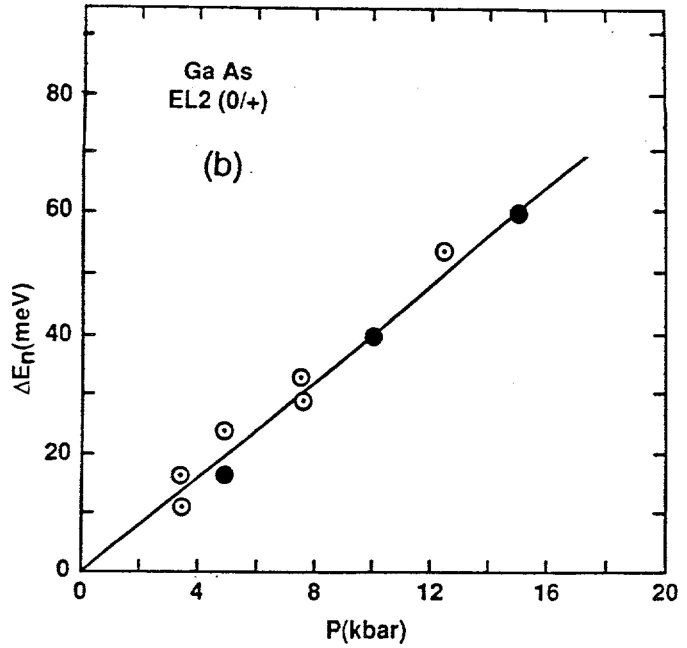
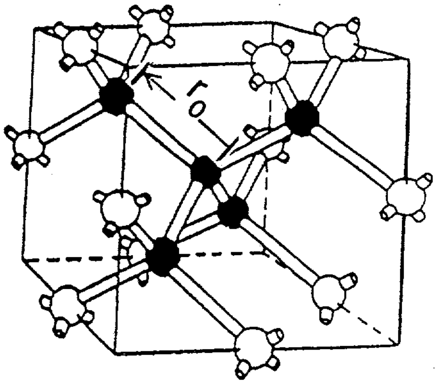
Pressure Results Support the Identification of EL2 as the Arsenic Autisite in GaAs





(c)	Relaxations $\Delta r/r_0$(%)	
	EL2 Experimental	As_{Ga} Theoretical
Defect Formation	+ 5.3	+ 7.7^a; + 4.9^b
(0/+) Transition	- 2.0	- 2.4^a
(+/++) Transition	- 3.3	

^{a}Chadi and Chang; ^{b}Caldas et al



(a) Normalized capacitance transients for electron emission from the (0/+) donor level of EL2 showing the large effect of pressure. The slope of each line is the emission rate at the indicated pressure and temperature.

(b) Pressure dependence of the thermal emission energy for the (0/+) transition of EL2.

(c) Comparison of our experimental lattice relaxations for EL2 and the theoretical values for the As antisite.

A New Technique has been Developed to Measure Complete Conduction and Valence-Band Dispersion Relations in Individual Strained-Layer Structures

by **E. D. Jones and S. K. Lyo**

Motivation — All of the important electrical and optical characteristics of a semiconductor, including bandgap energy, carrier effective masses, and carrier mobilities, can be determined once a detailed picture of the energy band structure of a material is known. This is particularly true in artificially-structured quantum wells or superlattice materials where compositions and layer thicknesses are intentionally varied to modify these parameters to obtain materials with the desired properties.

Accomplishment — A new and novel technique to measure simultaneously the energy band dispersion curves in a single sample of both the conduction and valence-bands in indium gallium arsenide (InGaAs)/ gallium arsenide (GaAs) strained quantum well (SQW) materials has been developed. These structures are important for high-performance n- and p-channel field-effect (FET) applications. The new technique utilizes a re-interpretation of the selection rules governing optical transitions in the low temperature (4° K) magnetoluminescence spectrum of such materials. For n-type SQW samples, the magnetoluminescence spectrum consists of transitions dependent upon the conduction-band/valence-band reduced mass and the conduction band mass. Under these conditions, a simultaneous determination of the conduction and valence-band dispersions is possible in single samples.

Significance — This new technique provides valuable experimental confirmation of theories that have been used to design these materials in the past. The technique also provides a nondestructive, noncontacting approach to the measurement of fundamental transport parameters of these SQW structures upon which efficient transistor or lasing action critically depends. This will provide a mechanism for fine-tuning the materials to optimize either FET or laser diode device performance.

Keywords: microelectronics, photonics, advanced materials, strained-layer superlattices

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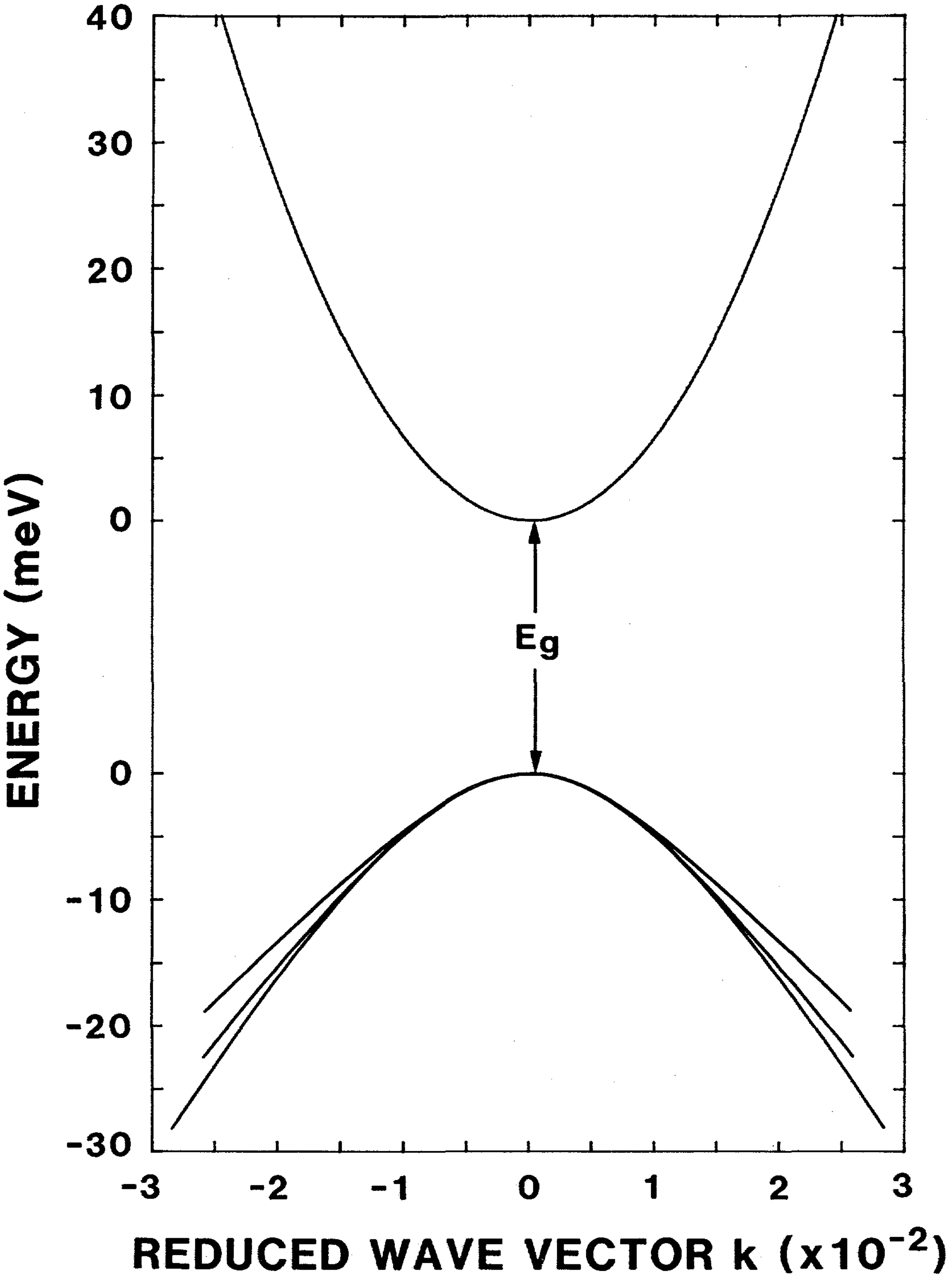
40
30
20
10
0
0
-10
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ENERGY (meV)
Eg
-3
-2
-1
0
1
2
3
REDUCED WAVE VECTOR k (x10⁻²)

Proof of the Existence of Phase Separation in InP$_{1\text{-}x}$Sb$_x$ Semiconductors Grown by Metal-Organic Chemical Vapor Deposition

by **R. M. Biefeld, K. C. Baucom, D. M. Follstaedt, and S. R. Kurtz**

Motivation — The rapidly growing field of optoelectronics is constantly looking for new materials with unique electronic properties for optoelectronic devices. One such material is $InP_{1-x}Sb_x$ which has been predicted to have bandgap properties appropriate for 2-5 μm infrared optoelectronic and certain heterojunction devices. Growth of this material by metal-organic chemical vapor deposition (MOCVD) and demonstration that its electronic properties meet theoretical predictions would be an important advance in the development of new photonic devices

Accomplishment — We have successfully grown $InP_{1-x}Sb_x$ by MOCVD, however we have discovered that a phenomena known as "phase separation" occurs in this material with a significant deleterious impact on the electronic properties relevant to optoelectronic device performance. Phase separation was discovered using a combination of x-ray diffraction, infrared spectroscopy, and transmission electron diffraction. We grew our $InP_{1-x}Sb_x$ films under a variety of conditions and then determined compositions of the samples with x-ray diffraction and electron microprobe techniques. In measuring the infrared properties of these materials (using photoluminescence, absorption, and photoconductivity), we found the peak energy of the photoluminescence occurred at lower energy than the previously reported bandgap for this material. The explanation for this result was revealed when we examined the material by transmission electron diffraction (see figure). This bright field image of an epitaxial layer of $InP_{0.68}Sb_{0.32}$ on InAs shows very fine modulation occurring along the $\langle 1\bar{1}0\rangle$ direction in sheets perpendicular to the (001) growth face. This type of modulation has been observed in other zinc blend materials and is thought to be due to a spinodal-like decomposition of the unstable alloy which results in a two dimensional phase separation. This explanation is supported by the optical spectra of the material which, in contrast to pure single phase alloys, display widely separated absorption and photoluminescence peaks (up to 0.5 eV difference).

Significance — The phase separation discovered in these $InP_{1-x}Sb_x$ alloys presents a significant challenge to the growth of novel materials for midwave (2-5) μm optoelectronic devices, far infrared detectors, and other projects which use metastable III-V semiconductors. Clearly, phase separated materials which exhibit the same poor optical and electronic properties we found in $InP_{1-x}Sb_x$ are not suitable for use in high quality infrared devices. In order to avoid poor quality devices, we must discover better growth conditions or use other compositions which eliminate or at least minimize the amount of phase separation.

Keywords: microelectronics and photonics, metal-organic chemical vapor deposition, infrared devices

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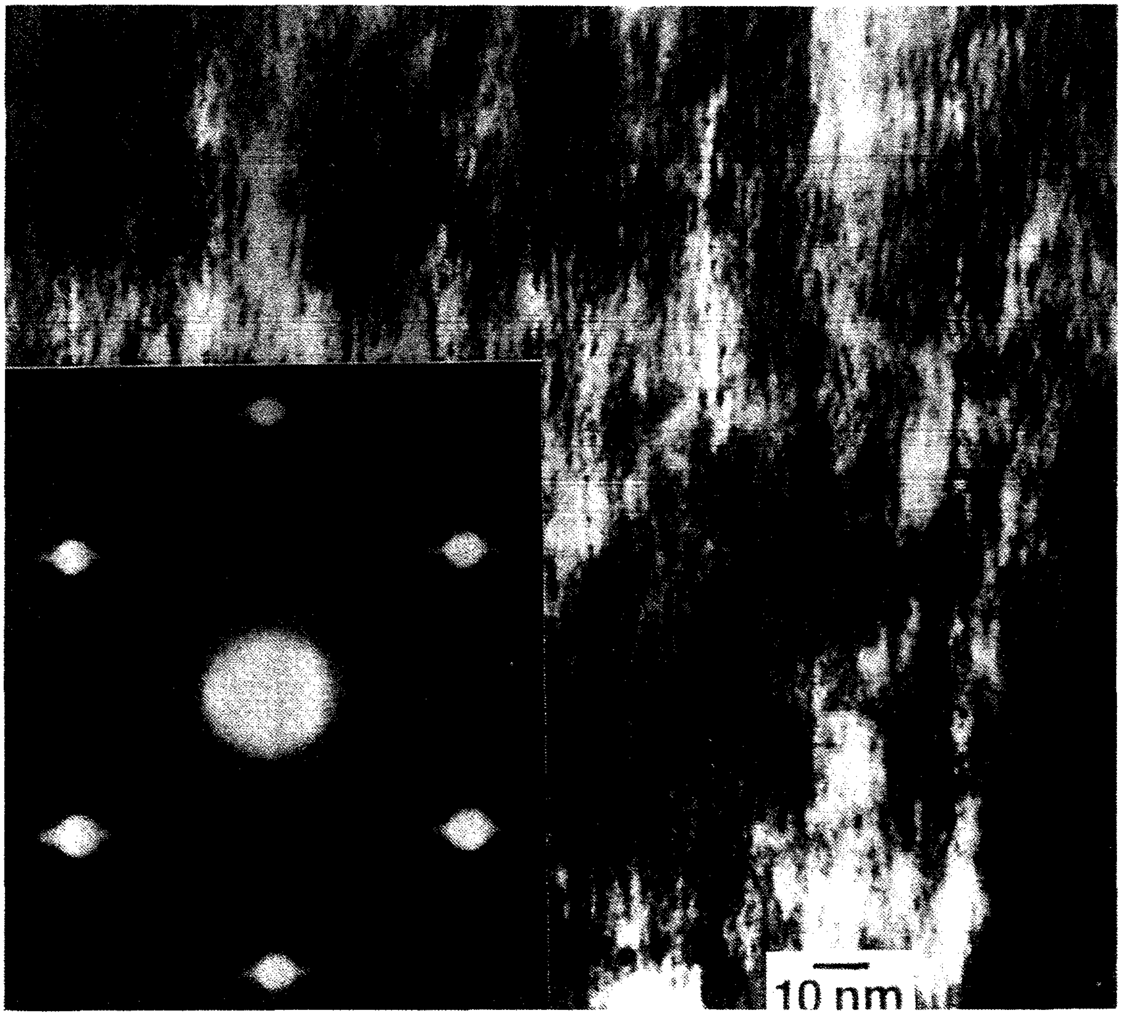
The decomposition of $InP_{0.68}Sb_{0.32}$ grown on InAs was identified by Transmission Electron Microscopy



The larger figure is a bright-field image showing modulations of the material into P-enriched and Sb-enriched phases (fine light / dark lines) separated by 2.5 nm. The inset is a <110> diffraction pattern showing intense reflections from the zincblende crystal structure surrounded by two weak "satellite" reflections which are caused by the modulation.

Compound Semiconductors are Passivated with ECR Silicon Oxynitride

***by* J. C. Barbour**

Motivation — Many microelectronic and photonic devices suffer from surface leakage and environmental or thermal degradation. The development of a low-temperature passivating layer can help alleviate these problems. Of immediate interest to Sandia is the passivation of InSb-based IR detectors, but such passivation can also be extended to GaAs. Currently, no technology exists to form high-quality passivating layers at room temperature, and conventional techniques often require high temperatures (>400° C) incompatible with InSb or GaAs. In this work, electron-cyclotron-resonance (ECR) plasma growth was employed to synthesize surface passivation layers on InSb and GaAs at room temperature. This goal was achieved through Sandia's unique position to utilize the cross-disciplinary fields in materials science of ECR-plasma growth, and compound semiconductor device processing and characterization.

Accomplishment—A novel growth process was developed for the passivation of InSb surfaces. Mixtures of SiH_4, N_2, and O_2 gases were used to grow high-quality SiO_xN_y dielectric films at temperatures from 30 to 250° C, downstream from an ECR plasma. The composition of the gas (and consequently the composition of the films) was critical for obtaining good surface adhesion on clean InSb. The film compositions varied from Si_3O_4N to Si_3N_4. The poor adhesion of Si_3N_4 on InSb (top figure) and the very good adhesion of Si_3ON_2 were explained in terms of thermodynamic driving forces for bond formation at the Si_3ON_2/InSb interface. The electrical quality of the passivation layers was characterized with capacitance-voltage (C-V) measurements over the frequency range from 500 Hz to 1 MHz (bottom figure). The Si_3ON_2 on InSb exhibited the best C-V characteristics consistent with long carrier lifetimes (~msec) and with a very low interface state density ~10^{11} /cm^2-eV. Also, the flatband voltage was approximately 0 V, which is important for potential applications in integrated circuits that must operate without an applied bias.

Significance — The basic understanding of the interfacial chemistry underlying passivation and adhesion is vital to implementing a technique compatible with device processing. This research lead to the first low temperature passivation process for InSb, which is expected to be transferred to industries dependent upon InSb-based devices. Interest from industry in the ECR process for GaAs passivation is beginning and is expected to lead to a CRADA in the next two years.

Keywords: microelectronics and photonics, passivation, InSb, GaAs, adhesion, ECR plasma

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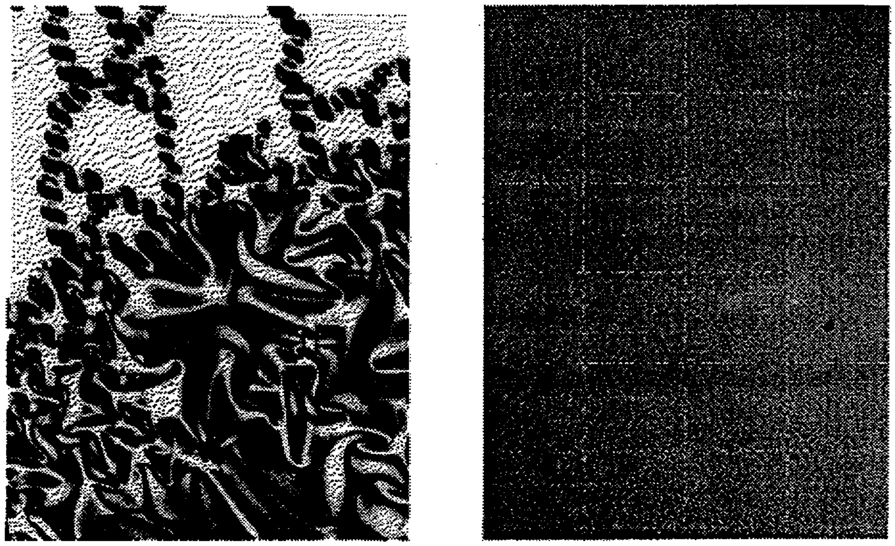
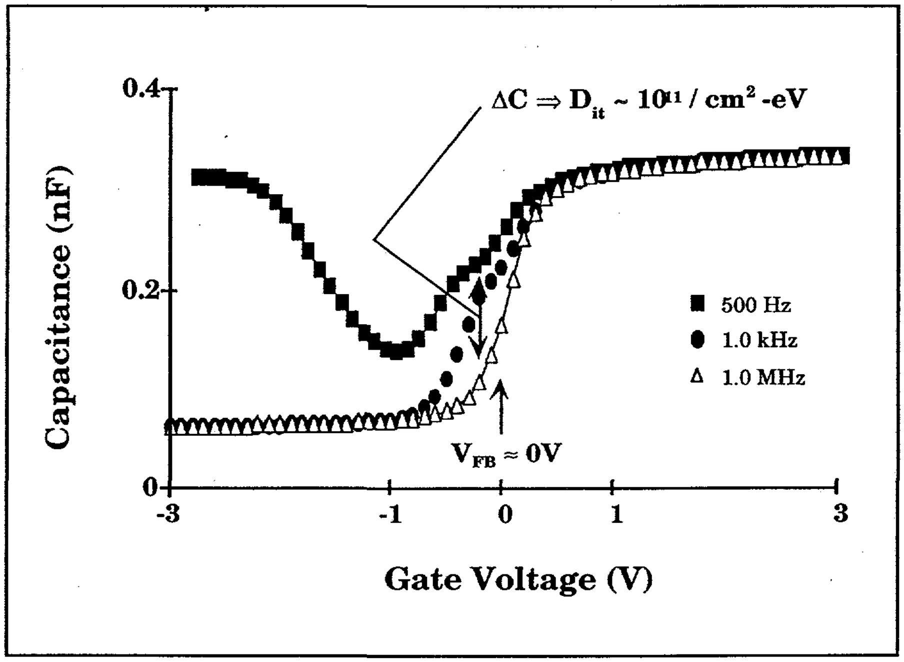
INTERFACE CHEMISTRY GOVERNS ADHESION PROPERTIES OF PASSIVATION LAYER



- Optical micrographs show de-adhesion of Si_3N_4 on InSb (left) and enhanced adhesion of Si_3ON_2 on InSb (right)

CV MEASUREMENTS AT 76°K SHOW HIGH-QUALITY DIELECTRIC PROPERTIES FOR Si_3ON_2/InSb



- ECR plasma growth achieves first low temperature (38°C) device-quality passivation of InSb (47nm thick).

- Slow recovery in inversion — ~msec lifetimes.

Rotating Disk Reactor Advances Our Understanding of the Chemistry Underlying Chemical Vapor Deposition

by **W. G. Breiland and M. E. Coltrin**

Motivation — Chemical vapor deposition (CVD) is a widely used technology for producing thin films for microelectronics, solar cells, protective coatings, and advanced materials. The chemistry of CVD is poorly understood -- successful processes have only been developed through laborious trial-and-error empiricism. The CVD industry needs fundamental physics and chemistry understanding to accelerate the development of new equipment and processes.

Accomplishment — We have used laser spectroscopy to measure the density of silicon atoms produced by gas-phase chemistry during the chemical vapor deposition of silicon from both silane and disilane. The experiments were performed in a high-speed rotating disk CVD reactor. Sandia has taken a leading role in developing this reactor as a well-characterized environment in which to study the chemical kinetics of CVD. For this reactor design, we have demonstrated that the fluid flow and temperature fields can be modeled precisely with numerical codes. These models can handle very complex chemical mechanisms.

Comparisons of the laser experiments with model predictions revealed that a different mechanism than was previously thought to occur significantly influences the loss of silicon atoms in the gas phase. The older mechanism failed to correctly predict several trends and silicon atom profile shapes observed in the laser spectroscopy experiments. After updating the chemical mechanism to reflect our new understanding of the kinetics of silicon atom production, we were able to adequately reproduce all trends and profile shapes for all experimental conditions.

Significance — Silicon is fundamental to the microelectronics industry. There remain unsolved manufacturing problems in silicon CVD such as deposition non-uniformities and gas-phase particulate formation that are directly related to the gas-phase chemistry of silane and disilane. A detailed understanding of the chemistry of these systems will help to solve manufacturing problems. In addition, this work clearly demonstrates the power of a well-characterized research reactor as tool for understanding the very complex physics and chemistry of CVD.

Keywords: chemical vapor deposition, microelectronics, photonics, advanced materials, numerical modeling

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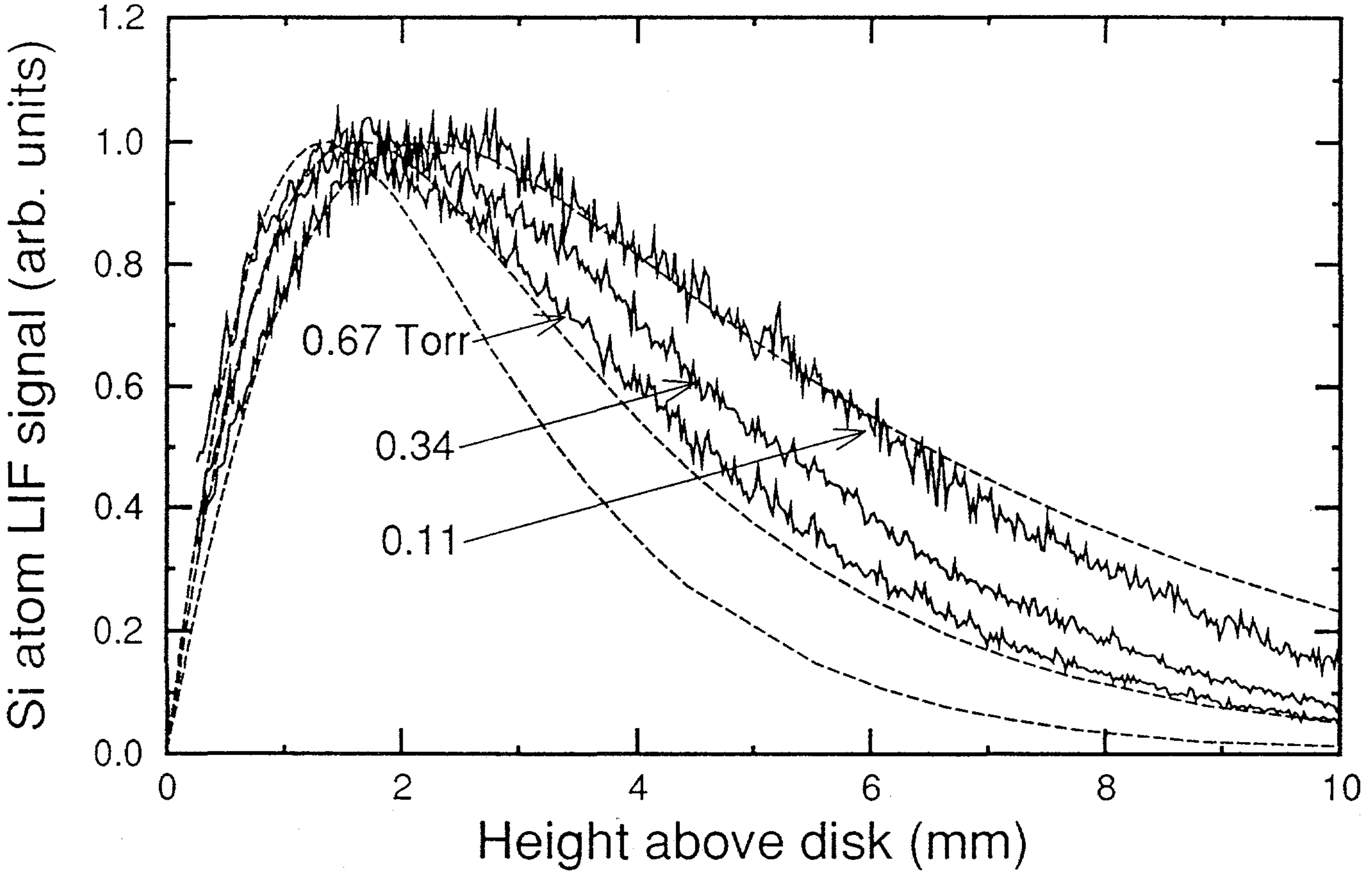
Comparison of Numerical Predictions with LIF Experiments of Silicon Atom Density for Three Partial Pressures of Silane



A Numerical Model has been Developed to Describe Diamond CVD

by **M. E. Coltrin**

Motivation — Diamond is a unique material due to it's properties of high thermal conductivity, hardness, and low coefficient of friction. The ability to grow diamond at atmospheric pressure and moderate temperatures by Chemical Vapor Deposition (CVD), rather than the previous high-pressure and high-temperature process, promises to open up many technological and consumer applications for diamond. However, CVD diamond must advance from the laboratory to applications through improvements in deposition quality, rate, and broad-area coverage. Development of predictive numerical models of diamond CVD will aid in process understanding and optimization. We are world leaders in modeling the chemically reacting flows occurring in CVD and have applied this unique expertise to diamond CVD. Currently there are four competing technologies for the CVD of diamond: DC-plasma arc-jets, microwave plasmas, hot-filaments, and combustion synthesis.

Accomplishment — We have developed detailed gas-phase and surface reaction mechanisms (containing 35 and 25 reactions, respectively) describing the decomposition of the hydrocarbon precursor, subsequent reactions of gas-phase products, and incorporation of species into the growing diamond film. We have also developed a numerical model (SPIN) for the coupled fluid flow, heat / mass transport, gas-phase and surface chemistry in rotating-disk or stagnation-flow CVD reactors. We have used the same reaction mechanism and modeling code to simulate all four of the deposition approaches mentioned above. The model predicts deposition rates, gas-phase temperature and velocity fields, and gas-phase species concentrations as a function of experimental parameters such as pressure, deposition temperature and reactant flow rate. Shown in the figure is a comparison of calculated and experimental (measured by W. L. Hsu, SNL/CA) chemical species concentrations at the deposition surface in a hot-filament reactor as a function of the amount of methane in the feed gas. Comparisons such as these verify the accuracy of our modeling approach.

Significance — We are collaborating with Norton Company to improve their DC-arc jet diamond deposition process. Our model is being used to understand the effect of varying process conditions on growth rate, uniformity, and film quality. It is being used to interpret the in situ measurements of Hsu in more fundamental studies of the chemistry in microwave-plasma and hot-filament diamond reactors. It is also being used to design and interpret a diamond combustion synthesis experiment being performed for an LDRD (by K. F. McCarty, SNL/CA). Our work in CVD modeling of Si CVD laid the foundations for our work on diamond CVD. It has been recognized through two BES Awards in Materials Chemistry (1984 and 1992).

Keywords: advanced materials, microelectronics, chemical vapor deposition, modeling

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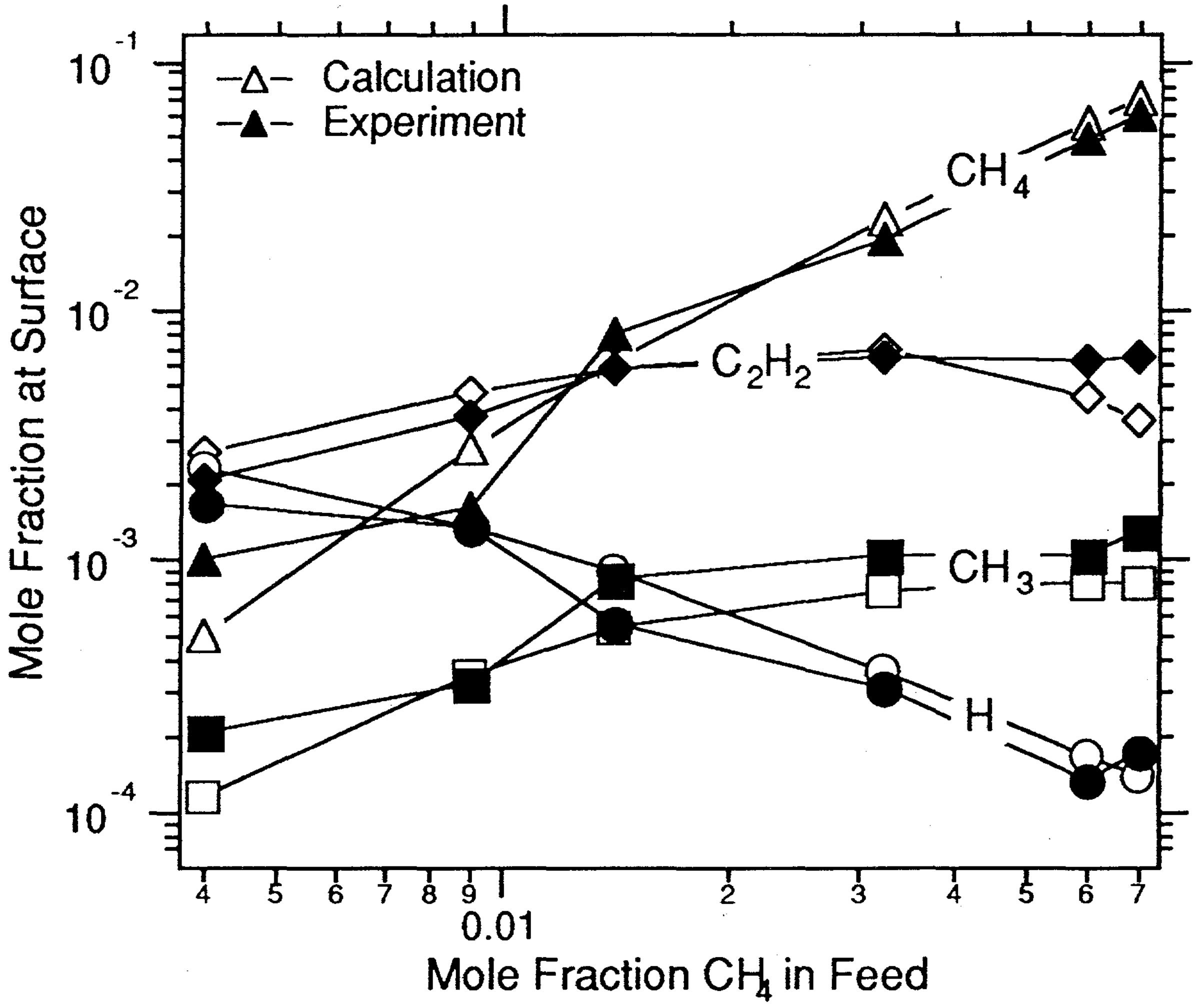
Model Predictions Match in Situ Measurements in Hot-Filament Diamond CVD Reactor



Tl-based Superconducting Ceramic Thick Films Carry Large Critical Currents

by **E. L. Venturini, M. P. Siegal, and J. A. Voigt**

Motivation — Three families of high-temperature superconducting (HTS) materials have been discovered with transition temperatures T_c above liquid nitrogen (77° K or -196° C). Most applications of these novel materials require a large lossless supercurrent at 77° K in moderate magnetic fields, but the maximum or critical current density J_c is sufficient only in single crystals or epitaxial thin films grown on lattice-matched substrate materials. Measurements on ceramic (polycrystalline) samples of these materials have shown disappointingly low J_c values due to problems at the grain boundaries. Some progress toward solving this limitation has been made with "textured" or partially oriented ceramics, but the processing involved is complex and not easily scalable to useful sample lengths. Hence, there is a requirement for a new, scalable process which yields a bulk ceramic with a large J_c. Recent progress has combined homogeneous, chemically prepared powders with simple screen printing and novel sintering techniques to produce thick films with sufficient J_c at low temperatures.

Accomplishment — The most promising HTS family contains the elements Tl, Ba, Ca, Cu, and O; two particular structural phases with nominal compositions $TlBa_2Ca_2Cu_3O_{8.5}$ (Tl-1223) and $Tl_2Ba_2Ca_2Cu_3O_{10}$ (Tl-2223) have T_c's of 120 and 125 K, respectively. These materials have been synthesized by starting with fully homogenized, mixed oxide precursor powders prepared by a patented solution chemistry technique. The powders were screen-printed as 20 μm thick films onto various substrates and sintered by an optimized rapid thermal process (RTP) cycle or in a two-temperature-zone furnace. Careful control of the TlO_x partial pressure was important during sintering. Both treatments yielded partially oriented ceramic material with attractive J_c values. The figure shows the maximum supercurrent I_c versus applied magnetic field at three temperatures flowing through a 0.5 cm wide, 20 μm thick Tl-1223 ceramic following RTP sintering. The I_c values were calculated from magnetization hysteresis data. At low temperatures, I_c exceeds 500 amperes in low fields and the modest decrease with increasing magnetic field indicates that the RTP process has greatly diminished the grain boundary problems. Thick films with these I_c values are very promising for several applications.

Significance — The demonstration of large critical current density in a relatively thick ceramic body represents a major step toward fabrication of practical wires and tapes based on high-temperature superconducting materials. Such wires are required for advanced energy applications such as more efficient motors and generators, HTS magnets and magnetic energy storage devices.

Keywords: energy efficiency, advanced materials, novel synthesis and processing, high-temperature superconductivity, critical current

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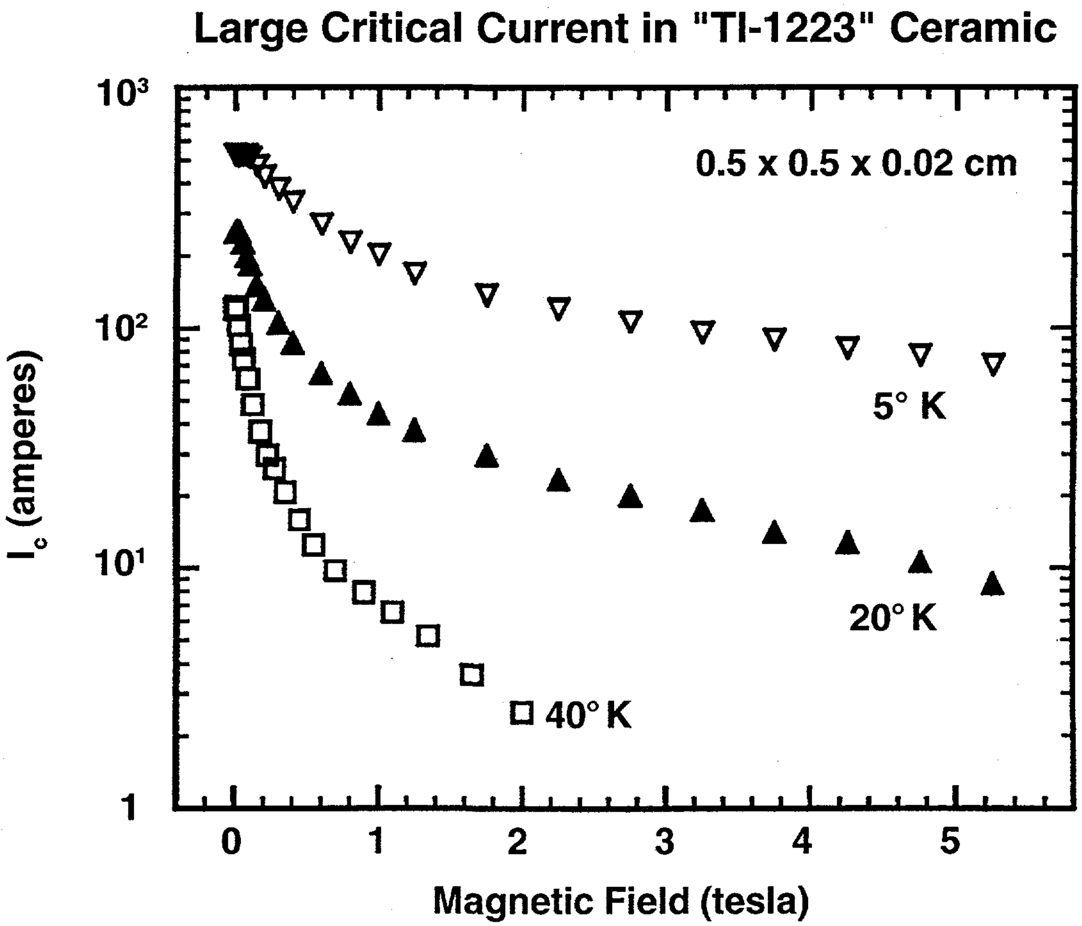

Figure Critical current I_c carried by a "Tl-1223" superconducting ceramic at 5, 20, and 40 K.

Broadband Light Emission is Observed from Fractal Quantum Wells

by **P. L. Gourley**

Motivation—Illumination sources are vitally important to human society. Each day, about 10 kilowatt-hours per person are dissipated to illuminate homes, offices, shops, schools, and vehicles. This adds to a total of to 2,500,000,000 kilowatt-hours dissipated in the United States alone! Only a small fraction of this power is useful. Most illumination sources are tungsten bulbs or fluorescent tubes. Tungsten bulbs produce 99.5% heat and 0.5% light, are inexpensive, but last only 2 years. Fluorescent tubes are more efficient (few percent) but use much phosphor which is toxic to humans and environmentally undesirable when disposed. Semiconductor materials can operate with 50 to 70 percent efficiency, last for decades, and can be disposed without harming the environment. Semiconductors which emit broadband light, as we have demonstrated, may have an important role to play in future illumination technology.

Accomplishment — We have synthesized a new, light emitting semiconductor material called a fractal quantum well. A schematic of the fractal quantum well, energy levels, and optical transitions is shown in the left side of Figure 1. Growth of the fractal material was accomplished by metal-organic vapor phase epitaxy of thin (~100 Å) layers of many different $Al_xGa_{1-x}As$ compositions. Luminescence from these new materials is highly efficient and can extend over a broad, selectable range of wavelengths as shown on the right side of Figure 1. The four spectra shown correspond to four different fractal sequences with layer thickness of 50, 100, 200, and 400. As the layer thickness increases, the luminescence increases in spectral bandwidth. In the thickest layer structures, the luminescence intensity is high and extends over a broad energy range of 300 meV.

Significance — We have produced a new class of efficient light-emitting semiconductor materials which borrow mathematical concepts found in nature. The materials are capable of emitting intense light over a broad range of wavelengths. This wavelength range can be extended into the visible range of the spectrum, making a white light emitting semiconductor possible. Such a light source could be used for illumination applications.

Keywords: semiconductors, quantum wells, optical properties, luminescence, illumination, fractals, naterials science

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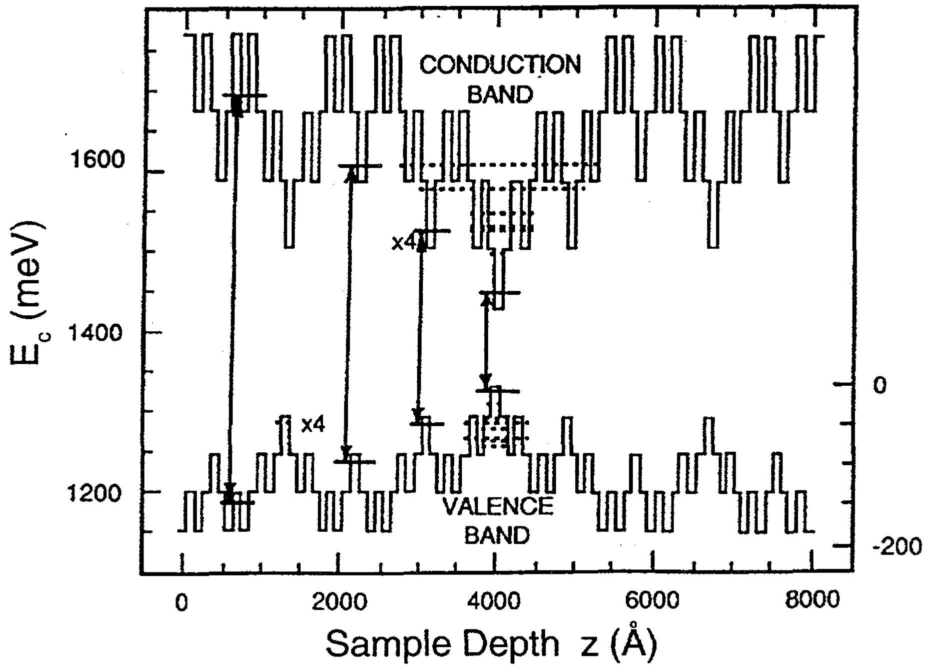
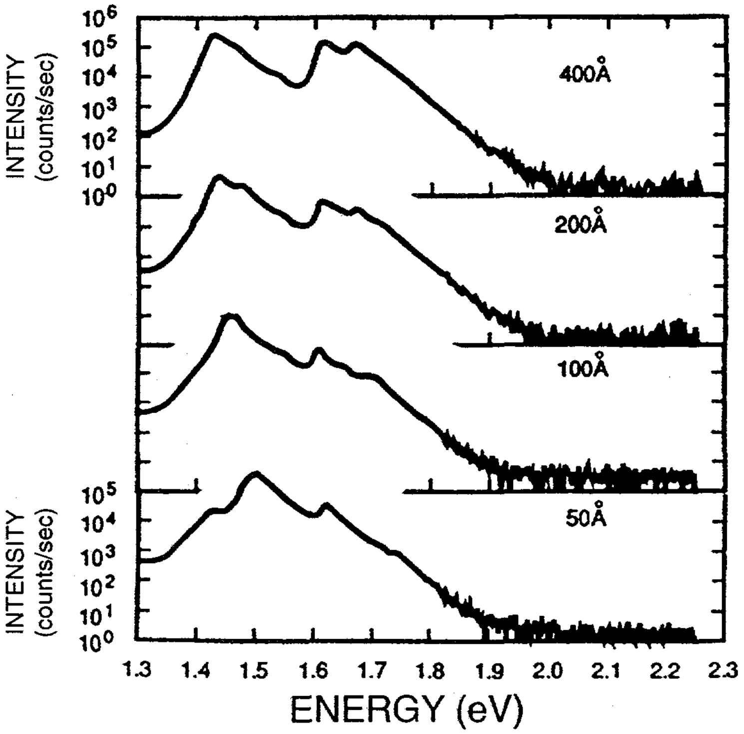
Band Structure Engineering using New Fractal Lattice Concept Demonstrated Broadband Emission in IR

AlGaAs Fractal lattice bandgap (theory)



Luminescence Spectra (experiment)



Potential new high effeciency white light source

New Pattern Recognition Technology from Vision Science Identifies Compounds and Classifies Cluster Features

by **G. C. Osbourn**

Motivation—Pattern recognition techniques use examples of data from patterns that are to be recognized (called training set data) to guess the identity of newly acquired data (called test set data). Such data can come from an enormous variety of problems. Examples include identifying hazardous chemicals in complex environments and classification of image features for satellite or biomedical applications. Many alternative pattern recognition techniques exist, but none perform in a way that competes with human visual perception. Improvements over existing pattern recognition performance are needed to adequately address many applications. The interdisciplinary capabilities in both vision science and physical/chemical sciences are well suited for successfully improving on existing technology.

Accomplishment—We have developed a new method for solving generic pattern recognition problems which is a major departure from previous techniques. The technique was developed by applying our newly achieved scientific understanding of human visual perception of patterns of data points to this problem. The result is an algorithm which mimics human performance and which provides several qualitative performance capabilities unavailable from existing methods.

Significance — We are now able to provide human-like pattern recognition performance to a variety of our customers for the first time. We are now partnering with microsensor specialists at SNL to develop effective chemical recognition software for their microsensor arrays with funding from a 1993 LDRD project. This chemical recognition technology will ultimately be applied to a number of Department of Energy and commercial sensing needs.

Keywords: pattern recognition, chemical sensing and recognition

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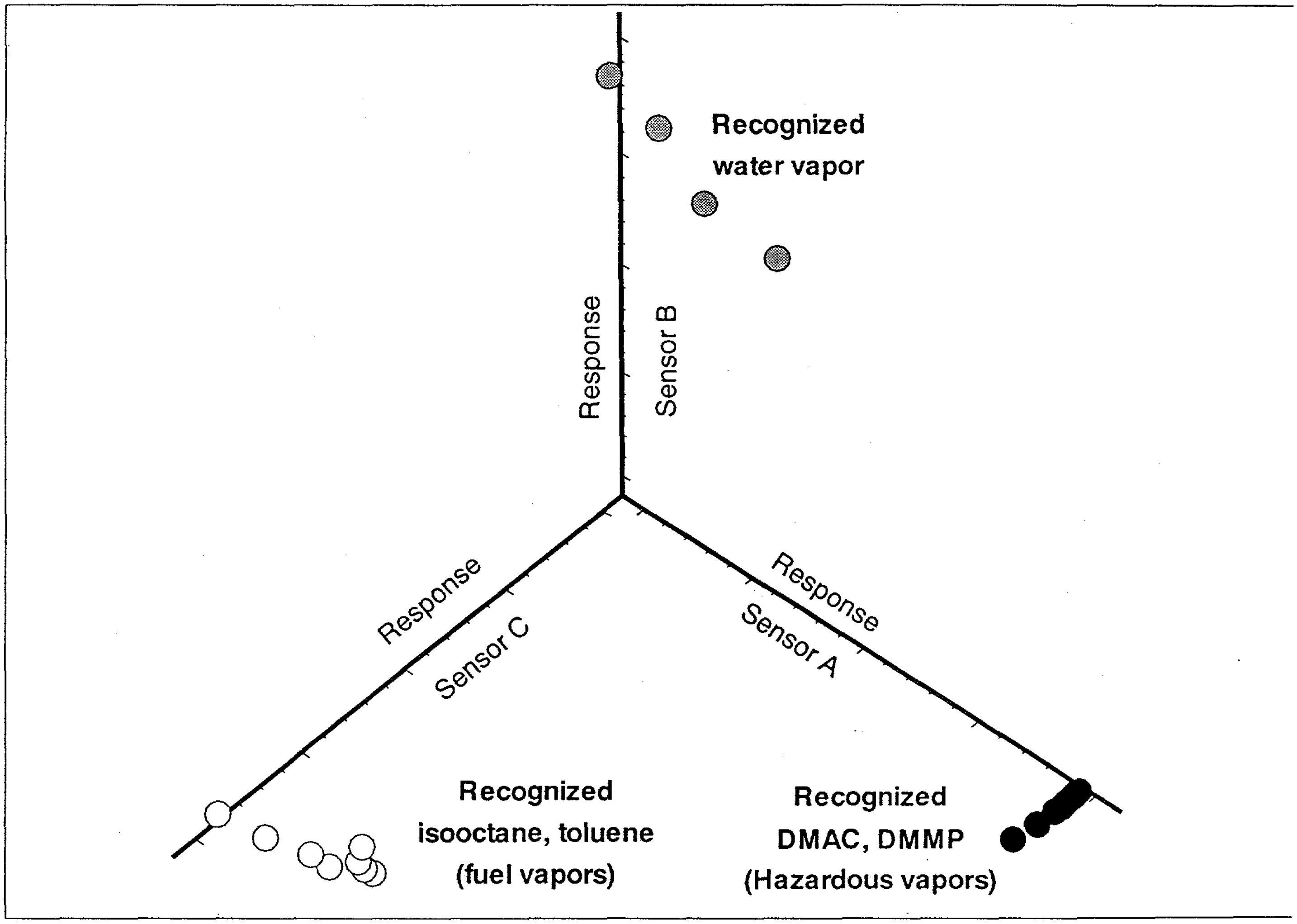
Hazardous and Background Chemicals are Distinguished by Applying Pattern Recognition to Multiple Sensor Signals



Application of pattern recognition technique to chemical sensing. The data are taken from the literature and are the responses of three chemical sensors to two hazardous chemicals and three background chemicals. Although the responses of individual chemical sensors are typically not specific enough to provide chemical recognition, pattern recognition of multiple sensor signals makes automated chemical recognition possible.

Multispectral Ultraviolet Fluorescence LIDAR Identifies and Maps Volatile Compounds in the Atmosphere

by **P. J. Hargis and G. N. Hays**

Motivation — Present techniques for mapping the concentration of volatile compounds in the atmosphere are either prohibitively expensive or nonexistent. Sandia National Laboratories is improving this technology through development of multispectral ultraviolet (UV) fluorescence Lidar (Light Detection and Ranging) technology. Improvements in the capability to generate real-time 3-D concentration maps of volatile compounds will have a major impact on atmospheric monitoring since today's mapping can require hundreds to thousands of samples and costly laboratory analysis.

Accomplishment — The advantages of multispectral UV-fluorescence Lidar technology rely on three critical components: (1) a database of dispersed fluorescence excitation spectra, (2) multivariate algorithms to analyze the spectra, and (3) a tunable UV all solid-state laser source. The technical viability of the multispectral UV fluorescence Lidar has been demonstrated in laboratory experiments which used an imaging fluorometer with an incoherent UV lamp in place of the tunable UV laser source. A typical dispersed fluorescence excitation spectrum from the chemical agent decay product pinacolone is shown in Figure 1. Multivariate algorithms developed at Sandia have been used to analyze such fluorescence spectra from mixtures of up to 12 compounds to correctly identify species at concentrations as low as 10 ppm. Based on our laboratory measurements and development of a tunable UV Optical Parametric Oscillator (OPO) laser source, identification of compounds at concentrations below 1 ppm-m in chemical clouds is feasible at distances in excess of 2 km.

Significance — Multispectral UV-fluorescence Lidar technology provides DOE with instrumentation that can generate 3-D concentration maps of volatile compounds released from DOE waste sites. In workplace settings using large quantities of volatile compounds, such as nuclear weapon assembly and dismantling, the technology also provides on-line workplace air-quality monitoring. The cost for DOE facilities to meet EPA regulatory requirements will be reduced by replacing costly point-monitoring technology with new technology that provides real-time, broad-area monitoring of volatile compounds in the atmosphere. Our work in this project has led to a patent disclosure on the laboratory fluorometer used to measure dispersed fluorescence excitation spectra.

Keywords: environmental compliance and restoration, nonproliferation and verification, process monitoring and control, intelligence, remote chemical speciation, LIDAR, tunable solid-state lasers, multivariate analysis algorithms, chemometrics

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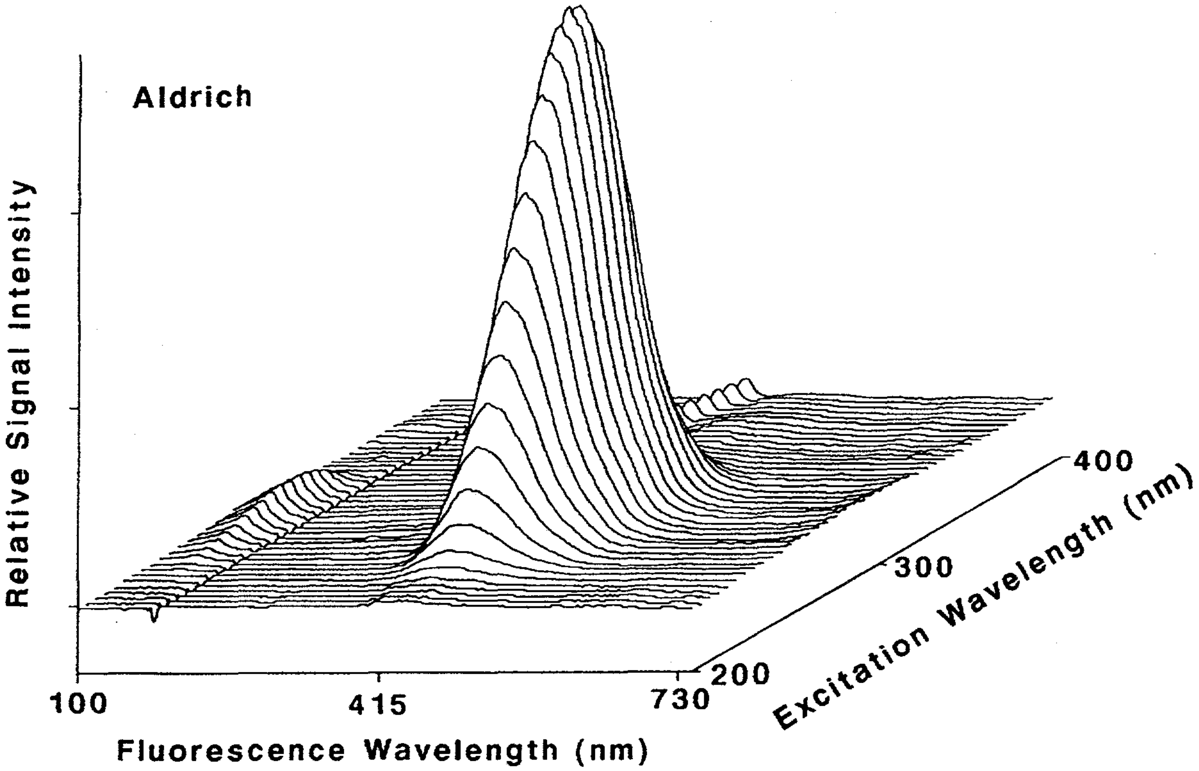
Pinacolone Fluorescence Excitation Spectrum



— Diagnostics and Characterization —

Materials Characterization

Our capabilities in this area include optical microscopy, scanning, electron microscopy, analytical transmission electron microscopy, double crystal x-ray diffraction, ion beam analysis of materials (RBS, channeling, ERD, PIXE, NRA), Hall measurements, photoluminescence, light scattering, electronic transport, deep level spectroscopy, magnetization, and dielectric and magnetic susceptibilities.

Chemical Vapor Deposition (CVD)

We have a wide range of experimental tools for investigating CVD which include optical probes for gas-phase and surface processes, a range of surface analytic techniques, molecular beam methods for gas/surface kinetics, and flow visualization techniques. Carefully chosen experiments provide the critical information on chemical species, gas temperatures, and flows necessary for model development and validation.

Surface and Interface Spectroscopies

We maintain strong capabilities in auger electron spectroscopy (AES), x-ray photoelectron spectroscopy (XPS), low energy electron diffraction (LEED), ultraviolet photoelectron spectroscopy (UPS), thermal desorption spectroscopy (TDS), infrared reflectance-absorbtion spectroscopy (IRAS), and quantum state resolved laser surface probes.

Sandia Nuclear Microprobe

The Sandia Nuclear Microprobe is used to study and evaluate the radiation hardness of microelectronic devices using two new advanced diagnostic techniques invented at Sandia: Single-Event-Upset Imaging and Ion-Beam-Induced-Charge-Collection Imaging.

Vision Science Laboratory

We have developed a vision science laboratory with state-of-the-art hardware and software capabilities for carrying out video inspection, multi-spectral image analysis, and sensor-based pattern recognition. These capabilities can be applied to applications ranging from microsensor-based chemical detection and recognition to automated video/SEM inspection of semiconductor materials and circuits.

Xternal Micro Ion Beam Analysis (X-MIBA)

This unique facility is designed for the multi-elemental analysis and ion irradiation of samples which are vacuum incompatible or extraordinarily large. Detection of elements ranging from all three isotopes of hydrogen to the transuranics is possible with sensitivities of 0.01 to 100 ppm.

Growth Science Laboratory

We have unique capabilities for in situ characterization of materials during molecular beam epitaxial growth, low energy ion bombardment on ion beam simulated growth using intensity profile sensitive reflection high energy electron diffraction (RHEED) for surface structure, energy dispersive x-ray reflectometry for in situ surface and interface structure, and Auger electron spectroscopy for surface composition.

KMAP X-Ray Diffractometer

KMAP X-Ray Diffraction Analysis is used to determine the lattice constant, strain relaxation, composition, layer orientation, and mosaic spread of a large variety of advanced epitaxial semiconductor materials.

Tandem Van de Graaff Ion Accelerator

This 6 MV EN accelerator provides ion species from hydrogen to bismuth for quantitative ion beam analysis of materials containing light elements (hydrogen to fluorine) using elastic recoil detection (ERD) and heavy elements using Rutherford backscattering spectrometry (RBS). This facility has also been used for high energy ion irradiation studies of high temperature superconductors.

Atomic-Level Imaging and Spectroscopy

We have developed unique capabilities in scanning tunneling microscopy (STM), field Ion microscopy (FIM), atom probe microscopy (APM), and interfacial force microscopy (IFM). Selected analysis is possible in both high temperature and ultra-high vacuum.

Resources and Capabilities in Physical and Chemical Science

Nanoelectronics Laboratory
We have capabilities for characterizing nanoelectronic structures (also fabricated at Sandia by e-beam lithography) through electrical transport measurements at low temperatures and high magnetic fields.

Lasers and Optics
We have extensive capabilities in characterizing and advancing the understanding in the area of solid-state lasers and non-linear optics, especially as coherent sources of broadly tunable light in rugged, compact geometries. We have established expertise in long-term and transient radiation effects characterization of optical materials.

Laser Spectroscopies
We have extensive capabilities for characterizing semiconductor materials by photoluminescence and magnetoluminescence down to low temperatures by optical laser imaging and laser microscopy, by laser excitation spectroscopy, and by time-resolved measurements of optical emission.

— Synthesis and Processing —

Nanocluster Laboratory
We have developed and patented a process based on the use of inverse micelles for the synthesis of large quantities of monodisperse clusters of metals, semiconductors, and oxides.

Electron Cyclotron Resonance (ECR)
This plasma facility has been built for studying fundamental processes governing the growth of oxide and nitride dielectric films used in optoelectronics and used as hard coatings.

400 kV Ion Implanter
This system is equipped with a variety of sources (gas, sputter, and metal vapor). This facility provides ion species from hydrogen to bismuth which can be used for studying fundamental irradiation mechanisms and selective chemical doping in semiconductors, ferroelectrics, and superconductors.

Molecular Beam Epitaxy
We have state-of-the-art commercial semiconductor growth laboratories for MBE growth of III-V and II-VI materials. In addition, we have research systems for Group IV semiconductor growth, including conventional and beam-enhanced epitaxial growth.

Metal-Organic Chemical Vapor Deposition (MOCVD)
We maintain state-of-the-art materials growth and characterization facilities with unique capabilities in MOCVD of compound semiconductor materials. Our facilities include commercial production MOCVD reactors as well as research reactors designed specifically for studies of CVD chemistry and for the development of advanced in situ diagnostics.

High Pressure and Shock Wave Physics and Chemistry Laboratories
Our capabilities in this area include large volume static high pressure apparatus which can be operated at temperatures ranging from 2° to 700° K and in magnetic fields; gas gun and explosive loading facilities with state-of-the-art, time-resolved diagnostics.

Shock Wave Synthesis
Recovery fixtures have been developed for use with gas gun and explosive shock loading facilities which allow unique material synthesis over broad ranges of shock pressures and temperatures.

Crystal and Thin Film Growth
Capabilities in this area include a pulsed laser deposition chamber, a thin film oxide deposition chamber, a diamond-like carbon deposition chamber, a hot filament chemical vapor deposition chamber, and various apparatus for single crystal growth.

Low-Temperature Plasma Analysis
We have state-of-the-art capabilities for the analysis of low-temperature plasmas as found in commercial processing reactors. These include emission spectroscopy, electrical characterization, laser and microwave-based measurements of species concentrations, electric field measurements (in situ), and others.

Resources and Capabilities in Physical and Chemical Science

— Theory and Simulation —

CVD Reactions
We have extensive capabilities to model complex chemically reacting flows such as occur in chemical vapor deposition manufacturing processes. Our numerical simulations can include the coupled gas-phase and gas-surface chemistry, fluid dynamics, heat, and mass transfer to provide predictive models of a chemical process.

Low-Temperature Plasmas
We have extensive capabilities in simulating the time and space evolution of low-temperature plasmas, focusing on new theoretical techniques for achieving rapid convergence and on direct comparisons with experimental results.

Optical Design
We have capabilities in novel optical designs, including resonators for application-driven laser geometries and in the application of binary optics. These capabilities are coupled to in-house micro-optics construction facilities and state-of-the-art optics testing.

Wave Propagation
We have developed advanced simulation codes for understanding wave propagation in optical parametric oscillators and amplifiers for the purpose of designing efficient, mission-oriented tunable laser sources.

Electronic Structure and Linear Scaling
Our capabilities in this area include First Principles Surface Impurity Code, a Pseudo-Potential Band Structure Code and the ability to perform total energy and full potential electronic structure calculations. We are also developing linear scaling algorithms to replace current algorithms which scale as the cube of the number of particles.

Semiconductor Calculations
Expertise in this area includes: Ab initio pseudopotential bandstructure, semiconductor transport and photoluminescence, Monte Carlo surface epitaxial growth and sputtering, and binary collision TRIMRC code to simulate ion-solid interactions. Workstations, CRAY-YMP, and massively parallel computational facilities are used.

— Recent Awards and Prizes in the Physical and Chemical Sciences Center —

1993 — American Physical Society International New Materials Prize to Gordon C. Osbourn, *"For originating the field of strained-layer superlattice electronics and optoelectronics by making the first theoretical calculations that predicted the unique electrical and optical properties of these materials and for inventing important new electronic and optical devices utilizing these properties."*

1993 — R&D 100 Award to David Ginley, Carol Ashby, and Tom Plut for *"Aqueous Chelating Etch System applied to High Temperature Superconductors."*

1993 — American Physical Society - Shock Compression Science Award to Robert A. Graham for *"In recognition of his major research contributions to the field of shock compression of condensed matter, especially his contributions to the understanding of the properties of shock compressed piezoelectrics, ferromagnetic, dielectrics, polymers, and semiconductors. In particular, his research on piezoelectric materials has led to the development of a family of highly reliable and widely used piezoelectric stress gages for time resolved measurements of stress wave profiles in shock loaded materials which have played a pivotal role in the study and understanding of shock phenomena."*

1992 — Department of Energy Materials Science Award for Sustained Outstanding Research to W. G. Breiland, M. E. Coltrin, G. H. Evans, P. Ho, and R. Kee for *"CVD Sciences."*

1992 — Department of Energy Materials Science Award for Sustained Outstanding Research to Barney L. Doyle, S. Tom Picraux, Jim A. Knapp, and Sam M. Myers for *"Advanced Ion Beam Techniques for Materials Analysis."*

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Recent Publications

Electric field inhibition and promotion of exchange diffusion on Pt(100), G. L. Kellogg, Phys. Rev. Lett. **70**, 1631 (1993).

Direct observations of atom migration in an externally applied electric field show that a positive field raises, and a negative field lowers, the activation barrier for the adatom-substrate atom exchange process. Above a critical field strength, the inhibition of exchange displacements is sufficient to change the diffusion mode from exchange to hopping. The field effect is explained by an electron-transfer process which changes the bonding of the adatom to neighboring surface atoms.

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The growth of InSb using alternative organometallic Sb sources, R. M. Biefeld, J. Crystal Growth, **128**, 511 (1993).

InSb is an important infrared material because of its small bandgap. It is also of interest for use in high speed circuit elements because of its low electron effective mass. We used alternate organometallic Sb sources, other than trimethylantimony, to achieve improved materials characteristics and enable lower temperature growth of InSb. The sources investigated were triisopropyl-, triethyl-, and tertiarybutyl-antimony as well as triethylindium.

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Linear response theory of inter-quantum-well tunneling in a double-well structure with in-plane magnetic fields, S. K. Lyo and J. A. Simmons, J. Phys: Condens. Matter **5**, L299 (1993).

A linear response theory of incoherent tunneling is presented and compared to data for the 2D-2D inter-quantum-well conductance for a double-well structure with an external in-plane magnetic field. The tunneling conductance, calculated by evaluating the current-current correlation function, shows resonances as a function of the magnetic field. The widths and heights of the resonance peaks depend sensitively on the intra-well scattering times and temperature. The theoretical results yield reasonable agreement with the tunneling conductance data.

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Computational simulation of diamond chemical vapor deposition in premixed C_2H_2 / O_2 / H_2 and CH_4 / O_2-strained flames, E. Meeks, R. J. Kee, D. S. Dandy, M. E. Coltrin, Combustion and Flame **92,** 144 (1993).

We have modeled combustion synthesis of CVD diamond in a stagnation-flow reactor under atmospheric conditions. In this configuration, a premixed flat flame flows over a flat deposition substrate that lies perpendicular to the flow and parallel to the burner face. Optimal growth conditions occur when the flame is lifted from the burner surface and stabilized at the deposition surface. The simulations include elementary gas-phase and surface agreement with observed growth parameters for the experimental conditions of Murayama, *et al*, who employed a premixed $C_2H_2/H_2/O_2$ gas mixture. Modeling CH_4/O_2 flame synthesis demonstrates that methane is less effective for diamond growth due to the decreased flame temperature and stability compared with C_2H_2 combustion.

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The mechanism of carbon incorporation during GaAs epitaxy, J. R. Creighton, B. A. Bansenauer, T. Huett, and J. M. White, J. Vac. Sci. Technol, **A4**, 1993 in press.

The use of trimethylgallium (TMGa) as the gallium source during epitaxial growth of GaAs often leads to high levels of carbon incorporation. Using temperature programmed desorption (TPD), high resolution electron energy loss spectroscopy (HREELS), and static secondary ion mass spectroscopy (SSIMS), we have identified a likely carbon incorporation pathway initiated by methyl group dehydrogenation. Methyl group dehydrogenation is evidenced by a small amount of hydrogen evolution around 430° C during TPD. Extended TMGa exposures in this temperature regime yield substantial coverages of methylene (CH_2) adsorbate which is detected by HREELS and SSIMS. The CH_2 adsorbate undergoes further reaction at higher temperature, yielding acetylene (C_2H_2), H_2, and CH_3 radicals as desorption products at ~550° C.

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Cover: The front cover of this edition features the new Integrated Materials Research Laboratory (IMRL) located at Sandia National Laboratories in Albuquerque, New Mexico. This 82,000 sq. ft. facility, scheduled for occupancy in 1994, will include state-of-the-art basic research facilities for tailored electronic and structural materials.