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OAK RIDGE NATIONAL LABORATORY

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SOLID STATE DIVISION

PROGRESS REPORT for Period Ending March 31,1997

MANAGED AND OPERATED BY
LOCKHEED MARTIN ENERGY RESEARCH CORPORATION
FOR THE UNITED STATES
DEPARTMENT OF ENERGY

ORNL-27 (3-96)

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ORNL-6934
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SOLID STATE DIVISION PROGRESS REPORT for Period Ending March 31, 1997

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Date Published – December 1997

Prepared for the
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Prepared by the
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37831
managed by
LOCKHEED MARTIN ENERGY RESEARCH, INC.
for the
DEPARTMENT OF ENERGY
UNDER CONTRACT NO. DE-AC05-96OR22464

Reports previously issued in this series are as follows:

ORNL-1095	Period Ending April 30, 1951
ORNL-1128	Period Ending July 31, 1951
ORNL-1214	Period Ending October 31, 1951
ORNL-1261	Period Ending January 31, 1952
ORNL-1301	Period Ending May 10, 1952
ORNL-1359	Period Ending August 10, 1952
ORNL-1429	Period Ending November 10, 1952
ORNL-1506	Period Ending February 10, 1953
ORNL-1606	Period Ending August 30, 1953
ORNL-1677	Period Ending February 28, 1954
ORNL-1762	Period Ending August 31, 1954
ORNL-1851	Period Ending February 28, 1955
ORNL-1852	Period Ending February 28, 1955
ORNL-1944	Period Ending August 31, 1955
ORNL-1945	Period Ending August 31, 1955
ORNL-2051	Period Ending February 29, 1956
ORNL-2052	Period Ending February 29, 1956
ORNL-2188	Period Ending August 31, 1956
ORNL-2189	Period Ending August 31, 1956
ORNL-2413	Period Ending August 31, 1957
ORNL-2414	Period Ending August 31, 1957
ORNL-2614	Period Ending August 31, 1958
ORNL-2829	Period Ending August 31, 1959
ORNL-3017	Period Ending August 31, 1960
ORNL-3213	Period Ending August 31, 1961
ORNL-3364	Period Ending August 31, 1962
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Acronyms

AES – auger electron spectroscopy
ANS – Advanced Neutron Source
APS – Advanced Photon Source
APECS – Auger-photoelectron coincidence spectroscopy
BCA – binary collision approximation
CCD – charge-coupled device
CDW – charge density wave
CHESS – Cornell High-Energy Synchrotron Source
CPA – constant-phase angle
CVD – chemical vapor deposition
DSC – differential scanning calorimetry
ECR – electron cyclotron resonance
EDX – energy dispersive x-ray
EELS – electron energy loss spectroscopy
EPR – electron paramagnetic resonance
FWHM – full width at half maximum
HFIR– High Flux Isotope Reactor
HPLC – high-performance liquid chromatography
HREM – high-resolution electron microscopy
HREELS – high-resolution electron energy loss spectroscopy
HRLEED – high-resolution low-energy electron diffraction
HRTEM – high-resolution transmission electron microscopy
HTSC – high-temperature superconductors
IBD – ion beam deposition
IPNS – Intense Pulsed Neutron Source
LDA – local density approximation
LEED – low-energy electron diffraction
MBE – molecular beam epitaxy
MOCVD – metallo-organic chemical vapor deposition
NSLS – National Synchrotron Light Source
ORISE – Oak Ridge Institute of Science and Engineering
PIGE – proton-induced gamma emission
PIXE – particle-induced x-ray emission
PLA – pulsed-laser ablation
PLD – pulsed-laser deposition
QMS – quadrupole mass spectrometer
RaBiTS – rolling-assisted biaxially textured substrates
RBS – Rutherford backscattering spectroscopy
RHEED – reflection high-energy electron diffraction
SANS – small-angle neutron scattering
SAXS – small angle x-ray scattering
SEM – scanning electron microscopy
SPEG – solid-phase-epitaxial growth
STEM – scanning transmission electron microscopy
STM – scanning transmission microscopy
TCR – thermochemical reduction
TDS – thermal desorption spectroscopy
TEM – transmission electron microscopy
TRR – time-resolved reflectivity
UHV – ultrahigh vacuum
UIUC – University of Illinois at Urbana-Champaign
WAND – wide-angle neutron diffractometer
WAXD – wide-angle x-ray diffraction
XDCD – x-ray double-crystal diffraction
XPS – x-ray photoemission spectroscopy
XRD – x-ray diffraction
YSZ – yttria-stabilized zirconia

Introduction

This report covers research progress in the Solid State Division from April 1, 1995, through March 31, 1997. During this period, the division conducted a broad, interdisciplinary materials research program in support of Department of Energy science and technology missions. The report includes brief summaries of research activities in condensed matter theory, neutron scattering, synthesis and characterization of materials, ion beam and laser processing, and the structure of solids and surfaces. An addendum includes listings of division publications and professional activities.

The past two years have been punctuated by the development of significant new opportunities for the division in neutron scattering and synchrotron x-ray research. A major upgrade of neutron scattering capabilities at the High Flux Isotope Reactor (HFIR) including a high-performance cold source, new beam lines and guides, and new and upgraded instrumentation is under way. These upgrades, together with the proposed Spallation Neutron Source at ORNL, will provide the nation with unsurpassed capabilities worldwide in neutron scattering. In addition, the division is also involved in the development of two synchrotron beam lines at the Advanced Photon Source at Argonne National Laboratory.

Theoretical progress has included new insights into thin-film and surface phenomena, highly correlated systems, and many body effects. Neutron scattering has seen continued growth in the scientific user program along with progress on a broad research front including superconductivity, magnetism, polymers and complex fluids, residual stress mapping, and improved instrumentation.

Advances in materials synthesis and processing are reported for superconductors, thin-film batteries, thermoelectrics, nanocrystals, and optical materials. Ion, laser, and molecular beam processing research has led to new understanding and control of defects, heterostructures, and thin-film growth. Significant progress has been made in the understanding of electrons at surfaces and in the evolution of surface morphology. New insights have been revealed on interfaces using atomic resolution scanning transmission electron microscopy and on electron correlations in metals using synchrotron x-ray scattering.

Many of these and other research advances over the reporting period have involved collaborations with more than 200 institutions worldwide, including Cooperative Research and Development Agreements with 13 industries and partnerships with The University of Tennessee, Vanderbilt University, and other universities and laboratories.

Chapter 1

Condensed Matter Theory

Surfaces and Grain Boundaries

ATOMISTIC PROCESSES IN THE EARLY STAGES OF THIN-FILM GROWTH[1]

Z. Y. Zhang and M. G. Lagally[2]

Growth of thin films from atoms deposited from the gas phase is intrinsically a nonequilibrium phenomenon governed by a competition between kinetics and thermodynamics. Once an adequate understanding of this competition is achieved, precise control of the growth and the properties of deposited films becomes possible. Considerable research activity has been focused on an atomic-scale understanding of this competition and has led to the discovery of many novel concepts. It is now recognized that the initial stages of film growth, albeit a very complex phenomenon, can actually be described by only a limited number of kinetic mechanisms, no matter what the growth mode or the deposition technique. These mechanisms include adatom diffusion on terraces, along steps, and around island corners; nucleation and dynamics of the stable nucleus; atom attachment to and detachment from terraces and islands; and interlayer mass transport. A recent review[1] has explored the importance of these kinetic mechanisms.

Descriptions of atomistic mechanisms of growth are based on the terrace-step-kink (TSK) model of a surface. Growth initiates with the deposition of atoms onto such a surface from the gas phase. On a complex substrate, an incoming atom may find it easier to reside at a shallower site at the earliest stages of adsorption and to travel a long distance before finding a stable site. A dimer, as the smallest island, is formed when two diffusing adatoms meet. Only islands larger than some critical islands are likely to grow. A stable island, such as a dimer, may still contain rich and intriguing dynamics (e.g., rotation and diffusion). A growing island will develop a fractal, dendritic, or compact shape, controlled by atom diffusion along island edges and across island corners. The morphology and distribution of the two-dimensional islands will greatly influence the subsequent (three-dimensional) growth of the film. Smooth growth can be achieved only with sufficient interlayer mass transport. Various ways have been identified to manipulate the growth kinetics in order to select a desired growth mode.

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1. Summary of paper: *Science* **276**, 377 (1997).
2. University of Wisconsin, Madison, Wis.

"ELECTRONIC GROWTH" OF ULTRATHIN METALLIC OVERLAYERS ON SEMICONDUCTOR SUBSTRATES[1]

Z. Y. Zhang, Q. Niu,[2] and C. K. Shih[2]

For both scientific and technological reasons, it is highly desirable to grow an overlayer on a different substrate with an atomically flat interface and growth front. However, it has not been possible to grow atomically flat overlayers in many heteroepitaxial systems. Fundamental obstacles to such smooth growth include stress effects because of lattice mismatch between the film and the substrate, kinetic limitations, etc. How to achieve smooth growth by suppressing growth instabilities has been the focus of film-growth studies.

In a recent study of Ag growth on GaAs(110),[3] smooth growth has been achieved above a critical thickness of seven monolayers (ML). The existence of such a critical thickness is unexpected. Theoretical effort aimed at understanding this important discovery has resulted in the formation of a conceptually new mechanism for smooth growth. In this mechanism, the influence of the quantum-well states in an ultrathin metallic overlayer on the stability of the overlayer is emphasized as the overlayer is placed on top of a semiconductor substrate. A systematic study of various metal/substrate systems reveals several distinct stability types, as characterized by the existence or absence of critical and magic thicknesses in the formation of atomically flat metal films. Depending on a delicate energy balance between a loss because of confinement and a gain because of charge spilling from the film to the substrate, the overlayer can be either stable above a critical film thickness or unstable for any thickness greater than 1 ML. Furthermore, if the interface-induced Friedel oscillations in electron density within the overlayer are sufficiently strong, an additional magic thickness for stable film growth can be defined.

This theory, termed as electronic growth, not only explains the existence of the critical thickness for Ag on GaAs, but also points to new directions for achieving smooth growth in many other systems. Some of its unique predictions are clearly supported by existing experiments. Efforts to establish fully the validity of this theory are likely to result in extensive theoretical and experimental activities in this field.

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1. Summary of paper to be published.
2. University of Texas at Austin, Austin, Tex.
3. A. R. Smith et al., *Science* **273**, 226 (1996).

DIMER SHEARING AS A NOVEL MECHANISM FOR CLUSTER DIFFUSION AND DISSOCIATION ON METAL (100) SURFACES[1]

Z.-P. Shi,[2] Z. Y. Zhang, A. K. Swan, and J. F. Wendelken

Diffusion of adatoms and clusters on surfaces is the most important kinetic process in thin-film growth. Since the invention of the field ion microscope and the scanning tunneling microscope, it has been possible to investigate surface diffusion down to the atomic scale. Of particular note is the diffusion of metal clusters on metal surfaces. Because of the relatively weak interatomic interactions involved, the mobility of such clusters is typically much higher than in any other systems, making the effects of cluster diffusion more significant. Therefore, recent attention has been focused on understanding the microscopic mechanisms of two-dimensional (2D) cluster diffusion in metal-on-metal systems.

Over the decades, the interpretation of all the experimental results from studies of cluster diffusion and dissociation on metal (100) surfaces has been based on the central assumption that cluster dynamics results from sequential motion of individual adatoms. This prevailing belief has been changed by a recent study[1] leading to the establishment of a novel atomistic process, dimer shearing. For all the model systems of homoepitaxially grown 2D clusters on fcc metal (100) surfaces, it has been found consistently that the sheared motion of a dimer (a bound pair of atoms) belonging to a small cluster always leads to orders of magnitude faster cluster dynamics than that induced by the motion of an individual atom. Dimer shearing is not only favored energetically, but its consideration also leads to an "entropic" gain along the diffusion pathway of a small cluster, as exemplified in Fig. 1 for the case of a tetramer. Furthermore, dimer shearing is a favored atomistic process for cluster diffusion even in heteroepitaxial systems, as long as the bulk lattice constant of the ad-cluster is smaller than that of the substrate.

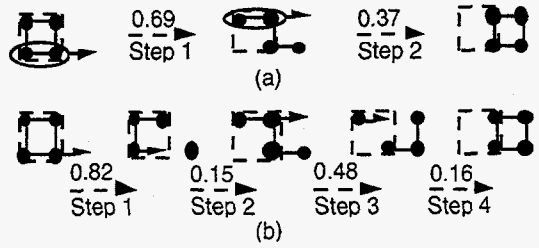

Fig. 1. Diffusion pathways and activation energies (in eV) for a Cu tetramer on Cu(100) via (a) dimer shearing and (b) sequential motion of individual atoms. The dashed squares mark the original place of the tetramer.

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1. Summary of paper: *Phys. Rev. Lett.* **76**, 4927 (1996).

2. ORNL/ORISE postdoctoral research associate. Present address: Read-Rite Corporation, Fremont, California.

EFFECTS OF HYDROGEN IN Ni(100) SUBMONOLAYER HOMOEPITAXY[1]

K. Haug,[2] Z. Y. Zhang, D. T. John,[2] C. F. Walters,[3] D. M. Zehner, and E. W. Plummer[4]

Surface impurities are nearly unavoidable in thin-film growth and are often unwelcome as they may easily degrade the quality of the films. Nevertheless, it has been discovered recently that the deliberate introduction of the right impurity into the growth front—a surfactant—can greatly improve the morphology of the films. Hydrogen is a common type of impurity in many thin-film growth systems. Its adsorption on the surface is often adventitious. This work presents a theoretical study of the effects of impurities on the formation, migration, and dissociation of two-dimensional islands of various sizes. It is partly motivated by the desire to understand microscopically how surface impurities can dramatically alter the mobility and/or the stability of adatoms, molecules, and islands. Such studies are also crucial for understanding why, in some circumstances, surface impurities can function as surfactants in enhancing layer-by-layer growth, while in many other cases they induce rougher growth.

The model system chosen for this study is H on Ni(100), and several fundamentally important issues are addressed by classical-potential total-energy calculations with semiclassical hydrogen zero-point-energy corrections. It is found that, when a H adatom encounters a Ni adatom, the two bind together with a weak attractive interaction, and the pair diffuses much faster than a single Ni adatom. H can also enhance the diffusivity of Ni by serving as a "stepping stone" for the Ni atom to hop over. Furthermore, when a H adatom reaches the edge of a Ni island, it can significantly increase the island mobility by reducing the kinetic stability of the island. Because these effects lead to a decrease in island density and a corresponding increase in island size, hydrogen will function as an anti-surfactant in Ni(100) homoepitaxy. Similar phenomena are expected to exist in other metal (100) epitaxial growth systems in which the diffusion of the host adatom is by normal hopping over bridges, as demonstrated experimentally for the case of Cu(100) homoepitaxy.

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1. Summary of papers: *Phys. Rev. B, Rapid Commun.* 55, R10233 (1997); in *Proceedings of the NATO ASI on Surface Diffusion: Atomistic and Collective Processes*, ed. by M. Tringides and M. Scheffler, Plenum Publishing Company, New York, in press.
2. Lehigh University, Bethlehem, Penn.
3. Graduate student from the University of Pennsylvania, University Park, Penn.
4. ORNL/UT Distinguished Scientist.

SIMULATION OF CHARGE TRANSPORT ACROSS GRAIN BOUNDARIES IN SILICON BICRYSTALS

R. P. Joshi[1] *and R. F. Wood*

Electrical transport in semiconductors can be greatly affected by grain boundaries (GB). Though the exact mechanisms are not yet fully understood, experimental work suggests that the GB electrical activity is predominantly extrinsic in origin. Oxygen in Czochralski Si is known to contribute significantly to GB electrical activity. The electrical characteristics are also known to depend on sample treatment and thermal history.

Electron transport in Si low-angle bicrystals has been analyzed by coupled Monte Carlo-molecular dynamics (MC-MD) simulations. The effects of discrete charges at the GB were studied and compared with results from one-dimensional treatments. The average charge density within the GB strongly influences transport characteristics, but the details of the charge arrangement itself are relatively unimportant. At low voltages, the currents are nearly an order of magnitude greater than those obtained from the simple thermionic emission model.

These results underscore the discrete nature of the GB charge distribution. Most previous studies, however, have assumed only one-dimensional potential variations perpendicular to the GB plane. To our knowledge, the only calculation that explicitly accounted for transverse fluctuations at a GB was by Mahan[2] based on a Markov averaging technique.

As an example of the types of results coming from the MJ-MD simulations, it was found that the current at 100 kV cm^{-1} for a GB charge, Qgb = 10^{11} cm^{-2}, is 5×10^4 cm^{-2} compared to 16.5×10^4 cm^{-2} without charge. As the external field was reduced to 10 kV cm^{-1}, J decreased substantially. At $Qgb = 10$ cm^{-1}, the 10-kV cm^{-1} field is barely sufficient to push electrons through the retarding barrier. After the initial velocity overshoot, a negative J results as the less energetic electrons from the swarm are repelled from the GB. For the 10^{11}-cm^{-2} case at 10 kV cm^{-1}, there is a small steady state current indicative of a "pinhole" effect. Reductions in the average distance between negative fixed charges at lower densities allow for a large fraction of the electron swarm to maneuver through pinholes between potential peaks.

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1. Old Dominion University, Norfolk, Va.

2. G. D. Mahan, *J. Appl. Phys.* **55**, 980 (1984).

DYNAMICAL SIMULATIONS OF NONEQUILIBRIUM PROCESSES—HEAT FLOW AND THE KAPITZA RESISTANCE ACROSS GRAIN BOUNDARIES[1]

A. Maiti,[2] G. D. Mahan,[3] and S. T. Pantelides[4]

A molecular dynamics simulation of the heat flow through a slab of silicon was made. The slab was periodic in the (x,y) plane, but had a thickness of 100 atomic planes in the z-direction. Two cases were reported: one for a single-crystal slab and the other with a low-index twin boundary at the midpoint of the slab. These results were the first reported simulations of heat flow in a solid.

Several technical problems had to be overcome in order to complete this project successfully. The first was to find a method of maintaining one face of the slab at a higher temperature than the other. This was done by damping particles in the cold face and speeding them up on the hot face. Another problem was to find a definition of a local temperature $T(z)$. The temperature was defined as the average kinetic energy of atoms in a slab parallel to the interface. A steady heat flow was modeled. By running the simulation for a long time, good statistics on the local temperature were obtained. For the case where the simulation was for a single crystal, the temperature was found to be a linear function of position between the two faces. This is the expected result, providing an important check on the accuracy of the simulation.

The most interesting case was where there was a twin boundary at the midpoint of the slab. The simulation showed a significant temperature discontinuity at this boundary. Such a temperature step is expected and is caused by the thermal boundary resistance. This is also called Kapitza resistance. The size of the temperature discontinuity was independently estimated by calculating the Kapitza resistance from phonon dynamics. The two methods gave the same result—molecular and phonon dynamics. This was the first simulation which showed a temperature discontinuity in a solid.

The results raise interesting physics questions. Some experts believe that heat is carried by the phonons in the solid. Temperature can only be defined on a scale of the average mean-free path of the system of phonons. In silicon, the phonons have a long mean-free path, which is longer than the thickness of the slab used in the simulation. These experts claim our results are meaningless since temperature cannot be defined on such a small scale of distance. Using this definition of temperature, as the average kinetic energy of atoms at an atomic site, the results appear quite reasonable. This has initiated a debate regarding the local definition of temperature.

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1. Summary of paper: *Solid State Commun.* **102**, 517 (1996).
2. ORNL/ORISE postdoctoral research associate. Present address: Molecular Simulations, Inc., Burlington, Mass.
3. UT/ORNL Distinguished Scientist.
4. ORNL Distinguished Visiting Scientist

ENERGY DEPENDENCE OF QUASIPARTICLE DAMPING AT A METAL SURFACE[1]

A. G. Eguiluz[2] and J. J. Deisz[3]

The dynamical properties of electrons in the vicinity of a metal surface are essential to a complete description of one- and two-photon photoemission, scanning tunneling microscopy, electron-scattering cross sections, etc. The usual theoretical schemes treat the electrons as moving in a static one-electron potential, such as the one which appears in density functional theory. This method often accounts for both occupied and empty-state electron energy levels accurately enough (i.e., errors are small on the eV scale that is typical of electronic bands). However, such a scheme does not reproduce an essential aspect of the corresponding quasiparticle excitations in dynamically correlated electronic systems; namely, the level widths, or lifetimes, of the actual electronic states.

Physical effects beyond the one-electron picture can be accounted for via an explicit evaluation of the non-local, energy-dependent electron self-energy $\Sigma(x, x)$ $|\varepsilon$, whose imaginary part embodies the physical processes contributing to the level widths. Numerical calculations of the energy dependence of the imaginary part of the self-energy at the surface of a simple metal, modeled by jellium, within the so-called *GW* approximation have been performed. This approximation includes the crucial physical effect of the dynamical screening of the electron-electron interaction; thus it is expected to be physically significant at least for weakly correlated metallic systems.

It was found that the energy dependence of $|m\ \Sigma$ is dominated by conventional ε^2 scaling for electron positions ranging from the bulk interior all the way to the jellium edge. However, non-quadratic contributions to $|m\ \Sigma$ become increasingly important, and eventually dominate, when the electron moves from the surface into the vacuum—at least down to energies on the order of $0.02\varepsilon_F$ above the Fermi level (closer to the Fermi surface, accurate numerical results for $|m\ \Sigma$ become difficult to obtain because of finite-size effects present in our slab simulations). This novel enhancement of non-quadratic contributions to the lifetime is interpreted as a signature of a dual surface-induced process: (1) states near the Fermi surface are frozen out as possible final states on the vacuum side of the interface, and (2) higher energy states have their probability amplitudes enhanced relative to their bulk counterparts.

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1. Summary of paper: *Phys. Rev. B* **55**, 9195 (1997).
2. UT/ORNL Collaborative Scientist.
3. Georgetown University, Washington, D. C.

QUANTUM BOLTZMANN EQUATION FOR PHOTONS AND DIFFUSION THROUGH A SLAB[1]

G. D. Mahan[2]

The quantum Boltzmann equation is derived for photons. It is interesting that this important equation was written over 100 years ago, and numerous solutions to it have been reported. However, the present derivation is the first ever of the equation itself. The derivation begins with the Hamiltonian for photons which includes their interactions with the material. Equations of motions are used to derive the time development of the distribution function for the photons. The Boltzmann equation is found by taking suitable frequency averages of these fundamental equations. Fundamental expressions are derived for the terms which absorb and scatter the photons. It is expected that the equation will be important in the theory of photon localization, because the derivation provides the framework for a description of localization.

Boltzmann's equation is solved exactly for the diffusion of photons through a slab. It is assumed that the slab scatters the photons strongly but does not absorb them. The boundary conditions are that the photons enter one side of the slab with normal incidence. Analytical expressions are obtained for the transmission and reflection intensities of the photons and for the angular distributions of the photons emitted from the front and back of the slab. This is the first exact solution for this important physical problem.

The solution can be applied to a wide variety of physical problems such as infrared diffusion of light through human tissue, light transmission through clouds, and light transmission through random media.

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1. Summary of papers: *J. Math. Phys.* **37**, 4333 (1996); *ibid* **36**, 6758 (1996).
2. UT/ORNL Distinguished Scientist.

DYNAMICS OF TWO-DIMENSIONAL TOPOLOGICALLY DISORDERED JOSEPHSON ARRAYS

M. Bartkowiak[1] *and G. D. Mahan*[2]

Two-dimensional Voronoi networks with a varying degree of disorder are used to model polycrystalline superconducting films. The superconducting grains, which are represented by space-filling Voronoi polygons of different sizes and shapes with a variable number of neighbors, are assumed to be coupled by resistively shunted Josephson junctions. At zero temperature and zero magnetic field, the current-voltage (*I-V*) characteristics of the networks parallel and perpendicular to the current and the current dependence of the number of vortex-antivortex excitations were calculated numerically. Values of the critical current of the networks appear to be very sensitive to the degree of the disorder. Depending on the applied dc current and on the disorder, voltages across the networks exhibit periodic, quasiperiodic, and aperiodic time dependences. The spatial distribution of the super current, the normal current, and the potential were also calculated, and the motion of vortices and antivortices in the network were simulated. For currents slightly above the critical current, *I-V* characteristics of disordered networks often resemble that of a single Josephson junction. In these cases, the potential distribution exhibits a cut along a single line in the network, and the vortex motion is confined to this line.

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1. ORNL/ORISE postdoctoral research associate.
2. UT/ORNL Distinguished Scientist.

SPONTANEOUS CHIRAL SYMMETRY BREAKING IN 2D AGGREGATION[1]

I. M. Sandler,[2] G. S. Canright,[2] Z. Y. Zhang, H. Gao,[3] and S. Pang[3]

Currently, there is much interest, both experimental and theoretical, in nonequilibrium growth processes and pattern formation. Recently, a Beijing experimental group discovered remarkable patterns in polycrystalline TCNQ (tetracyanoquinodimethane) and TCNQ-C_{60} aggregates, formed via nucleation and growth from thin amorphous films.[4] The films were deposited by the ionized cluster beam (ICB) technique. This technique has the important feature that it adds a small amount of net charge to the incoming beam.

The polycrystalline patterns are unusual in that they typically take the form of an "S" or "seahorse"-like shape. Besides being visually very striking, they also present a scientific challenge—they are either right- or left-handed (in roughly equal numbers), even though the molecules of which they are built and the crystals formed by these molecules are *achiral*. In all other known instances of chiral 2D aggregation (of bacteria, amphiphilic molecules, and vitamin C), the observed, macroscopic 2D chirality of the aggregates may be traced directly to the microscopic 3D chirality of the particles (bacteria or molecules) which form the aggregate. However in the case of the polycrystalline seahorses, the symmetry breaking is apparently spontaneous (i.e., not traceable to any microscopic source).

A growth model which makes essential use of the hypothesis that some of the charge incoming with the ICB beam is trapped on the growing polycrystalline aggregates has been conceived and studied. Simple electrostatics then forces this charge to be concentrated in the furthest tips of the growing body. The strong electric fields there then give higher growth, due to the attraction of the (mostly neutral, but polarizable) molecules in the matrix to regions of large electric field. Thus, there is a strong competition among growing branches of the aggregate. It was shown that this competition can give rise to growth histories in which an early dominance of one right (or left) branch gives rise to dominance of right (or left) branches at every subsequent branching event. The non-dominant branches then nearly stop growing, leaving fins on the outer edge of an S-shaped pattern which is qualitatively very much like the experimental seahorses.

As an important test of this picture, the Beijing experimental group performed ICB film-growth experiments[1] in the presence of an in-plane electric field. These experiments strongly corroborated the model; in both experiments and simulations with an in-plane field, the aggregates lost their curvature and grew predominantly along the direction of the field.

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1. Summary of paper to be published.
2. Guest Scientist from The University of Tennessee, Knoxville.
3. Chinese Academy of Sciences, Beijing, PRC.
4. H. J. Gao et al., *J. Mater. Res.* **9**, 2216 (1994).

FIRST-PRINCIPLES STUDY OF Se-INTERCALATED GRAPHITE[1]

J. O. Sofo,[2] M. Bartkowiak,[3] and G. D. Mahan[4]

The electronic properties and structure of selenium intercalated graphite are analyzed within the framework of density functional theory. This calculation is based on self-consistent energy band-structure calculations by the full potential linearized augmented plane wave (FLAPW) method. Se intercalated graphite compounds (GICs) are considered very promising candidates for room-temperature thermoelectric cooling devices. Se GICs in various stages have been produced recently at the University of Kentucky. Results show that there is no charge transfer between selenium and graphite. The energy of the $4p$ selenium orbitals, when intercalated in graphite, are close to the Fermi energy of the system and are mixed with the π band of the host. For low in-plane concentrations of selenium, these $4p$ selenium bands are flat and contribute to a high peak in the density of states. This peak, being right below the Fermi energy, explains the observed high thermoelectric power of this material. The nature of the bonding between Se and graphite layers and the position of Se atoms in the crystal structure were analyzed.

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1. Summary of paper: *Bull. Am. Phys. Soc.* **42**, 22 (1997).
2. ORNL/ORISE postdoctoral research associate.
3. UT/ORNL Distinguished Scientist.

Magnetism

SPIN DYNAMICS OF INCOMMENSURATE CHROMIUM ALLOY[1]

R. S. Fishman and S. H. Liu[2]

This work investigates the spin excitations of the incommensurate, antiferromagnetic spin-density-wave (SDW) state of pure Cr and its dilute alloys. Cr alloys are the prototypical transition-metal antiferromagnets, in which the conduction electrons are responsible for the antiferromagnetic behavior. Such systems are of great technological and fundamental importance. Depending on the concentration of impurities, the SDW of Cr alloys may be either commensurate (C) or incommensurate (I) with the bcc lattice. The I SDW state is modulated by the two wave vectors $Q\pm$ on either side of $G/2$ where G is a reciprocal lattice vector. Because $Q\pm \neq G/2$, the I SDW state has a different periodicity than the lattice.

Using realistic bands for the electron and hole energies, it was found that the spin excitations evolving from the SDW wave vectors $Q\pm$ consist of transverse spin-wave modes and longitudinal phason modes. While spin waves correspond to the rigid rotation of each spin about its equilibrium position, phasons correspond to the oscillation of the SDW back and forth along its wave vector direction. Phasons are predicted to bend toward the wave vector $G/2$ midway between the magnetic satellites and to produce the recently observed 60-meV peak in the longitudinal cross section at $G/2$. A new class of collective excitations called wavons is predicted to be associated with oscillations of the SDW wave vector. Wavons may be responsible for recently detected 15-meV peaks in the satellite cross sections. A final class of collective modes called amplitudons is associated with oscillations of the SDW amplitude at high frequencies. All four excitations are pictured in Fig. 1. Predictions are made for the temperature and doping dependencies of the phason- and wavon-mode frequencies.

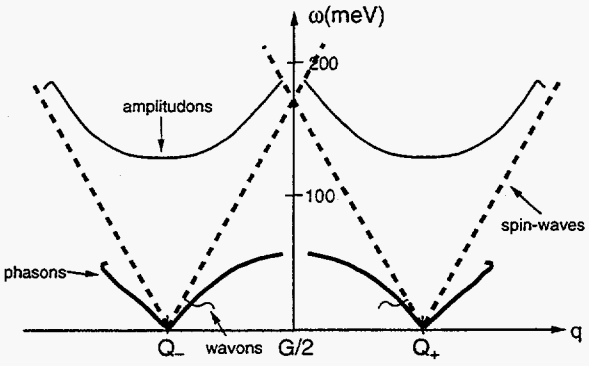

Fig. 1. The spin excitation spectrum of pure Cr at low temperatures.

This work provides the first fundamental understanding of the dynamical behavior of transition-metal antiferromagnets. New types of excitations have been introduced to describe the complex dynamical behavior of these prototypical systems. Guided by these results, future experiments may achieve a better understanding of the spin-wave, phason, and wavon excitations.

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1. Summary of papers: *Phys. Rev. Lett.* **76**, 2398 (1996); *Phys. Rev. B* **54**, 7233 (1996); *Phys. Rev. B* **54**, 7252 (1996).

2. University of California–Berkeley, Berkeley, Calif.

3. T. Fukuda et al., *J. Phys. Soc. Jpn.* **65**, 1418 (1996).

CHARGE DYNAMICS OF CHROMIUM ALLOYS[1]

V. S. Viswanath[2] and R. S. Fishman

While the spin dynamics of Cr alloys have been extensively investigated both experimentally and theoretically, no experiments have yet been performed on the associated charge dynamics of Cr alloys, and theoretical results are lacking. This work evaluates the charge dynamics associated with the CDW in Cr alloys. The charge excitation spectrum is found to contain three classes of excitations including phason modes. Using the random-phase approximation, the cross section of the charge phasons is evaluated. With the availability of modern high-flux synchrotron sources, it should now be possible to perform the necessary inelastic scattering measurements. Such measurements would constitute the first observation of the CDW dynamics in a bulk system.

Previous work on the spin dynamics of Cr alloys revealed the presence of four classes of excitations: spin waves associated with fluctuations in the polarization direction, phasons related to translational oscillations, wavons connected to oscillations in the ordering wave vectors $Q\pm$, and amplitudons associated with fluctuations in the SDW amplitude. Both spin waves and phasons are Goldstone modes which have zero frequency at the SDW ordering wave vectors. By contrast, phasons are the only Goldstone modes that contribute to the charge dynamics. These modes evolve from the ordering wave vectors $2Q\pm$ of the CDW, on either side of the reciprocal lattice vector G. Although spin waves are absent, both wavons and amplitudons are also expected in the CDW excitation spectrum. All three types of excitations are shown in Fig. 1.

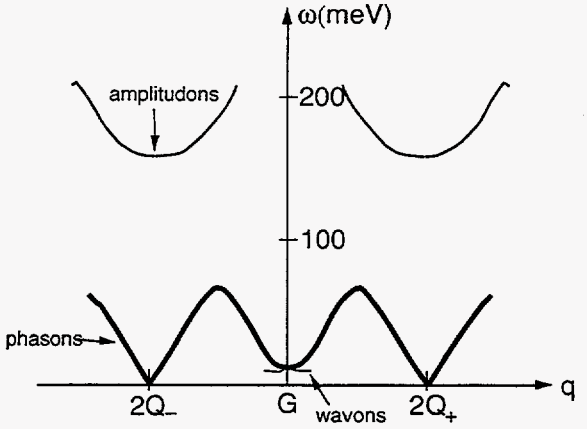

Fig. 1. The charge excitation spectrum of pure Cr at low temperatures.

The phason modes are damped for any nonzero frequency. Midway between the CDW satellite wave vectors $2Q\pm$ and the reciprocal lattice vector G, the charge phasons have zero slope and an enhanced x-ray scattering cross section. Estimates for this cross section range from 10^3 to 10^4 counts/s, assuming that the Bragg peak intensity is 10^{10} counts/s. Consequently, the cross section of the charge phasons should be large enough to observe using modern synchrotron sources. Measurements of the charge phasons in Cr alloys would constitute the first observation of the CDW dynamics in a bulk, three-dimensional system.

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1. Summary of paper: *J. App. Phys.* **81**, 4204 (1997).
2. Postdoctoral research associate from North Dakota State University, Fargo, N. Dak.

COUPLED SPIN- AND CHARGE-DENSITY WAVES IN CHROMIUM ALLOYS[1]

R. S. Fishman and X. Y. Jiang[2]

In addition to a spin-density wave (SDW), Cr alloys are also known to contain a charge-density wave (CDW) with twice the SDW wave vector. Both the SDW and CDW are produced by the Coulomb attraction between electrons and holes on two nested Fermi surfaces. This work investigates the effects of the CDW on the phase transitions between the paramagnetic (P), commensurate (C), and incommensurate (I) states of the SDW. While the C SDW state of CrMn and CrFe alloys has the same periodicity as the atomic lattice, the I SDW state of pure Cr and CrV alloys has a different periodicity than the lattice. The CDW is shown to produce both the weak first-order PI transition found in pure Cr and the strong first-order PC transition observed in CrFe and CrSi alloys.

While the SDW in Cr can be observed from the strong neutron scattering intensities at wave vectors $\pm Q$, the CDW appears in x-ray scattering[3] measurements as satellite peaks at wave vectors ± 2, on either side of the reciprocal lattice vector G. Both the SDW and CDW develop below the Néel temperature T_N, which is 310 K for pure Cr. Over a wide range of temperatures below T_N, the CDW amplitude is proportional to the square of the SDW amplitude.

This model uses realistic quasiparticle energies within the random-phase approximation to determine the effects of the CDW. Several previously unexplained phenomenon are attributed to the CDW. First, the observed discontinuity in $dT_N dx$ (x is the impurity concentration) at the triple point is caused by the presence of a CDW in the I phase. Second, the strongly first-order PC transitions in CrFe and CrSi alloys are associated with the growth of a large CDW in the I phase of those systems. An experiment is proposed to verify this claim. Third, the CDW has important effects on the order and slope of the IC phase boundary. Finally, this work goes beyond the Landau-Ginzburg expansions used in previous work to find the effect of the CDW on the weakly first-order PI transition of pure Cr.

This research is the first to evaluate the effect of the CDW on the magnetic phase diagram of Cr alloys. Because Cr alloys are the prototypical transition-metal antiferromagnets, these results are of great fundamental significance.

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1. Summary of papers: *J. Appl. Phys.* **81**, 4201 (1997); *J. Phys., Condens. Matter.* **9**, 3417 (1997).
2. North Dakota State University, Fargo, N. Dak.
3. J. P. Hill, G. Hegelsen, and D. Gibbs, *Phys. Rev. B* **51**, 10336 (1995).

COMPETITION BETWEEN SPIN-DENSITY WAVE AND MAGNETIC COUPLING IN Fe/Cr MULTILAYERS[1]

Z.-P. Shi[2] and R. S. Fishman

Fe/Cr multilayers have been studied extensively over the past 10 years since the discovery that the multilayer resistance is greatly reduced by the alignment of the Fe moments. This behavior, called giant magnetoresistance, has various potential applications in sensor devices. Despite many experimental studies, however, the competition between the bulk spin-density wave (SDW) ordering in Cr and the magnetic coupling between Cr and Fe at the multilayer interfaces has been poorly understood. Because the SDW wave vector of pure Cr and its dilute alloys is incommensurate or has a different period than the atomic lattice, the properties of Fe/Cr multilayers can potentially be controlled by modifying the SDW wave vector with doping. A model was developed to understand this competition and the effect of the SDW ordering on the properties of Fe/Cr multilayers.

This simple model assumes the magnetic interactions at the Fe-Cr interface to be antiferromagnetic and adds the bulk-free energy of the Cr spacer obtained from many-body theory. When the Cr spacer is sufficiently small or the temperature sufficiently large, the SDW is shown to become commensurate with the same period as the atomic lattice. Recently, these commensurate-to-incommensurate transitions were observed experimentally.[3,4] Hence, this model explains the magnetic phase diagram of Fe/Cr multilayers as a function of Cr thickness and temperature. With increasing Cr thickness, the model predicts that the SDW alternately stretches to satisfy the interfacial Fe/Cr coupling and then contracts closer to the lowest energy configuration of bulk Cr. A spin switch is proposed to stabilize either the commensurate or incommensurate SDW phases by flipping the Fe moments.

This work provides a simple model for the behavior of the SDW in a Fe/Cr trilayer or multilayer. It provides a guide for future experiments to probe the complex behavior of these materials. Because the SDW of Cr can be controlled with doping and temperature, Fe/Cr multilayers may prove to have even greater industrial applications than other multilayers with nonmagnetic spacers.

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1. Summary of paper: *Phys. Rev. Lett.* **78**, 1351 (1997).
2. ORNL/ORISE postdoctoral research associate. Present address: Read-Rite Corporation, Fremont, Calif.
3. A. Schreyer et al., *Europhys. Lett.* **32**, 595 (1995); A. Schreyer et al. (unpublished).
4. E. E. Fullerton, S. D. Bader, and J. L. Robertson, *Phys. Rev. Lett.* **77**, 1382 (1996).

CANTED MAGNETIC COUPLING IN Fe/Cr MULTILAYERS[1]

Z. P. Shi,[2] Y. Wang,[3] G. M. Stocks,[3] D. M. C. Nicholson,[4] W. A. Shelton,[5] O. Yasar,[6] and Z. Y. Zhang

Magnetic coupling in magnetic multilayers can manifest itself in a variety of ways. When the magnetization orientation between two adjacent magnetic layers across a nonmagnetic spacer is ferromagnetic or antiferromagnetic, the coupling is bilinear. Bilinear coupling is commonly interpreted in terms of the RKKY interaction or within a quantum-well picture. In addition to bilinear coupling, there exists experimental evidence for magnetic multilayers having 90° coupling, referred to as biquadratic coupling. The corresponding mechanism suggested for biquadratic coupling involves spatial fluctuations in the bilinear coupling, which is extrinsic in nature, caused by roughness at the interfaces or magnetic impurities in the spacers. For multilayers with spacers whose bulk properties show antiferromagnetism, in-plane non-collinear (NC) coupling may exist, especially for systems with reduced interface roughness.

A recent study[1] has reported the first *ab initio* calculation of general magnetic configurations in Fe/Cr(001) multilayers, using the locally self-consistent multiple scattering method. The direction and magnitude of the magnetization of each monolayer in the magnetic multilayer are obtained. A more general, "canted," coupling is found between the Fe layers. The canted coupling, as depicted in Fig. 1, can be decomposed into a NC component in the film plane and an out-of-plane component. The canting can be attributed to the intrinsic itinerant antiferromagnetic nature of the Cr spacers, which themselves are in a spiral spin configuration. The canted coupling picture obtained in this study can be compared with available experimental data when proper projections to specific planes or directions are made.

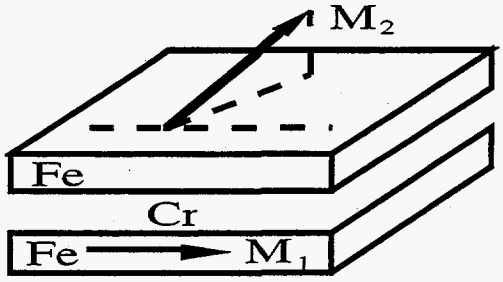

Fig. 1. Canted magnetic coupling between two Fe layers mediated by a Cr spacer.

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1. Summary of paper: *Phys. Rev. Lett.* (in press).
2. ORNL/ORISE postdoctoral research associate. Present address: Read-Rite Corporation, Fremont, California.
3. Metals and Ceramics Division, ORNL.
4. Computational Physics and Engineering Division, ORNL.
5. Computer Science and Mathematics Division, ORNL.
6. Center for Computational Science, ORNL.

EXCHANGE AND CORRELATION LOCAL-FIELD CORRECTIONS TO THE RESPONSE FUNCTIONS OF A SPIN-POLARIZED ELECTRON GAS[1]

D. C. Marinescu and J. J. Quinn[2]

In a study of an interacting electron system, the concept of a local-field correction originates in the deviation of the effective potential experienced by an electron from the mean-field value. Exchange (x) and correlation (c) effects associated with the short-range Coulomb repulsion are responsible for a change in the density in the vicinity of each electron, the exchange-correlation hole, which acts as a perturbation on the rest of the system.

When an imbalance in the up and down spin populations is created by a static magnetic field, local-field corrections beyond the random phase approximation are described by spin-dependent functions, $G^x{}_\sigma{}^c$. The self-consistent response of this system to a weak electromagnetic perturbation—an electric potential and a magnetic field of arbitrary orientation—consists of coupled charge and longitudinal spin fluctuations, as well as transverse magnetization in respect to the initial direction of polarization.

The equation-of-motion method for a time-dependent distribution function was used to derive microscopic expressions for $nG_\sigma(\omega)$. Because of the interaction, the solution for the one-particle distribution depends on the two-particle correlation function, which at its turn satisfies an equation of motion that includes three-particle correlations. The infinite chain can be cut off in the limit of large wave vectors or high frequencies, when it is assumed that the three-particle interaction is negligible in respect to the Coulomb repulsion. In this case, an analytic solution which gives the local-field factors in terms of the two-particle correlation function in equilibrium is possible.

Results show that the local-field corrections are not only spin dependent but also that they have different expressions for the longitudinal and transverse magnetic response. For large wave vectors, G_σ can be expressed in terms of the two-particle correlation function, $g_{\sigma,\sigma'}(\mathbf{r})$ at $r = 0$, and depends only on the initial degree of polarization of the system.

The correct wave vector and frequency dependence of the local-field factors are useful in determining the excitation frequencies of the collective modes of the system, defined as the poles of the response functions. These excitations correspond to interband transitions which can be determined experimentally from Raman absorption spectra. By comparing the experimental data with theoretical predictions, different models for the many-body interaction can be tested.

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1. Summary of paper to be published.
2. Guest scientist from The University of Tennessee, Knoxville, Tennessee.

ORIGIN OF HIGH-ENERGY STRUCTURE FOUND IN INELASTIC NEUTRON SCATTERING EXPERIMENTS

J. F. Cooke and J. A. Blackman[1]

Recent neutron scattering experiments at the ISIS facility at the Rutherford Appleton Laboratory have yielded more evidence in support of the itinerant-electron theory. Persistence of the lower branch of the spin-wave dispersion curve out to the Brillouin boundary in nickel, predicted by theory but not previously observed, was located. Although the data have not been fully analyzed, considerable structure was also observed at high energies near the zone boundary. Theoretical calculations of the spin part of the inelastic scattering intensity were made.

The obvious source of such structure is in the part of the cross section that was not calculated, the orbital part. Calculation of the orbital term, even within the random phase approximation, is very difficult. As an initial step, the orbital scattering has been calculated for the noninteracting case. If structure is found similar to that observed, a more detailed calculation would be warranted.

Results from such calculations of the orbital part of the cross section along the 100 direction for ferromagnetic nickel and iron are shown in Fig. 1. There is considerable structure in both cases. Similar results were found for scattering along the 110 and 111 directions. A comparison with experiment will be made as soon as the fully analyzed data from the measurements at ISIS are made available. If the orbital term is found to be the source of the structure observed in the high-energy ISIS measurements, then neutron scattering should provide an important new test for the band structure of transition-metal ferromagnets.

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1. University of Reading, Reading, United Kingdom.

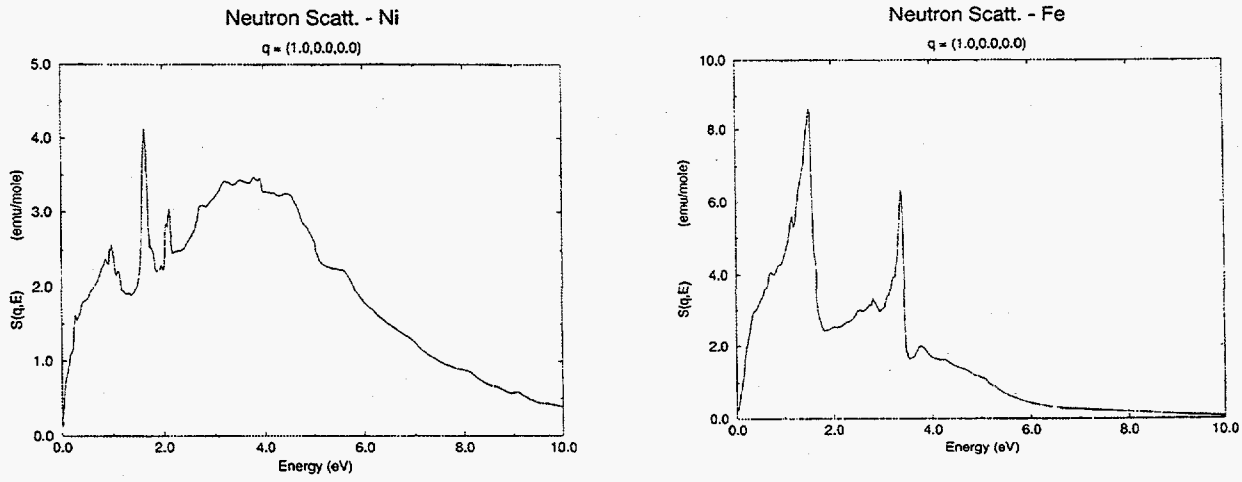
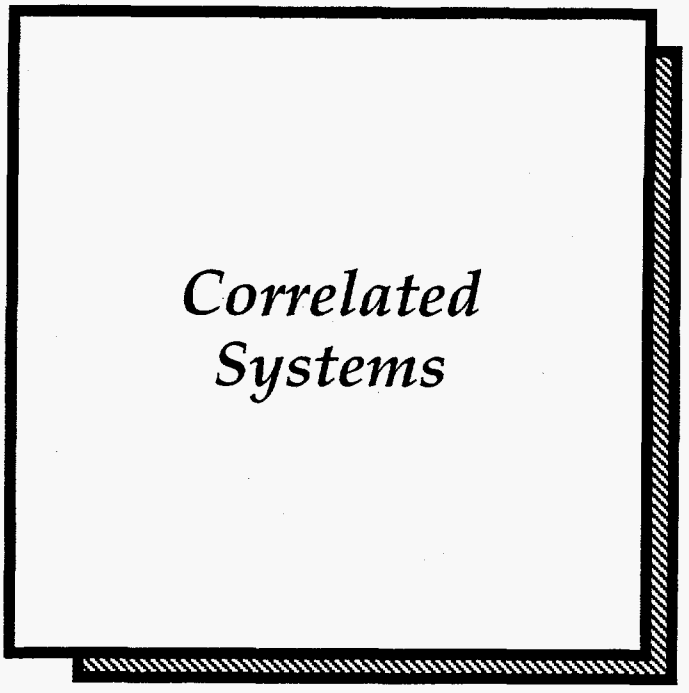


Fig. 1. Orbital scattering at the 100× zone boundary for nickel and iron, respectively.


Correlated
Systems

ONE-ELECTRON EXCITATIONS, CORRELATION EFFECTS, AND THE PLASMON IN CESIUM METAL[1]

A. G. Eguiluz,[2] R. Stumpf,[3] and A. Fleszar[4]

The measured plasmon dispersion relation of the heavy alkali metals (Rb and Cs) is in complete disagreement with textbook physics. In effect, the dispersion is *negative* for small wave vectors[5] and is anomalously flat for large wave vectors. This situation was initially viewed as a signature of the presence of strong correlations—in a system which has traditionally been regarded as a "simple" metal.

The dynamical electronic response of Cs at a first-principles level was studied. The calculations were performed in two stages. The first stage started from a local density approximation (LDA) band structure obtained with use of an *ab initio* pseudopotential in which the 5*p* shell is assigned to the core. These calculations established that the negative dispersion is due to the effect of one-electron transitions into a complex of final states which is nearly degenerate with the plasmon energy.

In the above calculations, the polarizability of the core was excluded (by construction), and thus the theoretical dispersion curve is too high for small wave vectors. The second stage of our calculations with the construction of a pseudopotential in which the 5*p* orbitals are treated as valence states. It was found that these spatially localized states induce a physical interplay between crystal local fields and electronic correlations, leading to a novel, and relatively large, many-body (downward) shift of the plasmon energy ω_p. This effect, combined with that of the one-electron transitions into empty states close to ω_p, yields a dispersion curve which is in excellent agreement with experiment for small wave vectors. In addition, these results feature a flat dispersion for large wave vectors, in qualitative agreement with experiment.

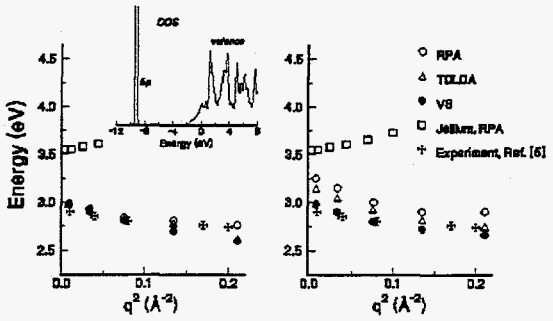


Fig. 1. Plasmon dispersion relation in Cs for small wave vectors along the (110) direction. The 5*p* semi-core states are treated as valence states. Right (left) panel includes (ignores) the crystal local fields. Theoretical curves are labeled by the vertex correction used in the respective calculation. Inset: calculated density of states.

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1. Summary of paper: *Phys. Rev. B* 55, 2068 (1997).
2. UT/ORNL Collaborative Scientist.
3. Sandia National Laboratories, Albuquerque, N. Mex.
4. Universität Würzburg, Würzburg, Germany.
5. A. vom Felde, J. Sprösser-Prou, and J. Fink, *Phys. Rev. B* 40, 10181 (1989).

THE ELECTRON SELF-ENERGY IN METALS: CONSERVING CALCULATIONS IN THE SHIELDED-INTERACTION APPROXIMATION[1]

A. G. Eguiluz[2] and W.-D. Schöne[3]

A full description of the dynamical properties of electrons in a metal requires solution of the many-body problem of interacting electrons in the presence of the periodic array of ions in which they are embedded. This is a formidable problem for which only partial solutions are known.

A numerical evaluation of the electron self-energy in simple metals within the shielded interaction approximation (SIA) has been performed. As formulated by Baym and Kadanoff, the SIA has the virtue that it fulfills all microscopic conservation laws and that it includes the crucial effect of dynamical screening. Computations of the self-energy from renormalized propagators dressed with the same self-energy were evaluated. It was found that many-body self-consistency—which has traditionally been ignored—has a significant impact on the chemical potential, the quasiparticle weight at the Fermi surface, and the spectral weight of the satellite in the density of states. Of course, the SIA ignores other effects (e.g., ladder diagrams) whose importance needs to be assessed on an equal footing (i.e., self-consistently). This has never been done for realistic models of metals.

These results were obtained by the implementation of finite-temperature many-body techniques which are applicable for realistic band structures and more general self-energy functionals. These techniques are similar—but not identical—to field-theoretic methods developed recently for models of highly correlated electrons in two dimensions. In Fig. 1, the impact of one of the key elements of our algorithms, which is designed to obtain accurate Green's functions on the imaginary-time axis from the updated Green's function at the Matsubara frequencies, is illustrated. The dressed polarizability is then evaluated by fast-Fourier-transform techniques. The real-w quantities are obtained by Pade approximants.

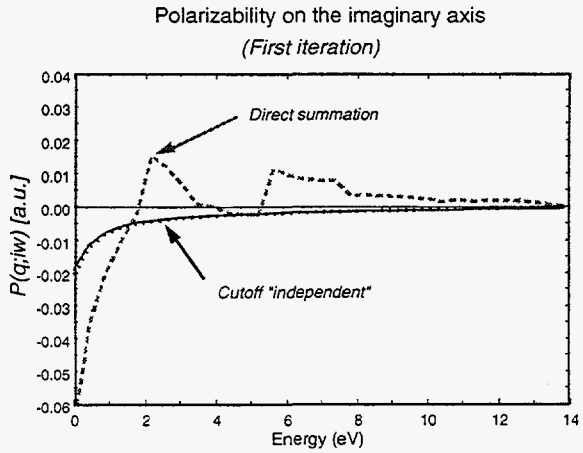

Fig. 1. Polarizability on the imaginary frequency axis. Dashes: obtained from $G(q,\tau)$ computed by direct summation over $G(q,i\omega_n)$ with a frequency cutoff of 14 eV. Dots: results obtained upon calculating $G(q,\tau)$ taking into account the behavior of the Fock diagram at large frequencies; same cutoff is used. Solid line: exact result—indistinguishable from the former, on the scale of the figure. Here $r_s = 5$, $q = 0.32\ k_F$.

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1. Summary of paper to be published.
2. UT/ORNL Collaborative Scientist.
3. Postdoctoral research associate from The University of Tennessee.

CORRELATION ENERGY AND ITS TEMPERATURE DEPENDENCE[1]

S. Hong[2] and G. D. Mahan[3]

Electron-electron interactions play an important role in determining the properties of metals. Many calculations have been done on the influence of electron-electron interactions on metallic properties such as cohesion, transport, optical response, and magnetism. Very few of these calculations have been done at nonzero temperatures.

In reviewing the few previous calculations of the temperature dependence of the cohesive energy of metals, it was realized that serious errors had been made. The present calculation is the first correct calculation of the temperature dependence of the correlation energy of the electron gas for the case which included only ring diagrams. This is usually called the "random phase approximation." Many of the results were expressed as a power series in the ratio $t = k_B T / E_F$, where k_B is Boltzmann's constant and E_F is the Fermi energy of the electron gas. The first nonzero term in the expansion is proportional to $O(t^2)$. Numerical results were presented for the coefficient of the t^2 term for the correlation energy. The temperature dependence of the exchange-correlation potential was also calculated. This latter function could be used in calculations of the temperature dependence of the local density approximation. The first correct results for the temperature dependence of this potential were presented.

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1. Summary of paper: *Phys. Rev. B* 53, 1215 (1996).
2. ORNL/ORISE postdoctoral research associate. Present address: Metal and Ceramics Division, ORNL.
3. UT/ORNL Distinguished Scientist.

EXCLUSION STATISTICS FOR FRACTIONAL QUANTUM HALL STATES ON A SPHERE[1]

S. B. Isakov,[2] G. S. Canright,[3] and M. D. Johnson[4]

Previous work[5] has established that the quasiparticles in the fractional quantum Hall effect (FQHE) obey a fractional exclusion principle in Hilbert space. For example, addition of a single quasielectron near the FQHE state $\upsilon = 1/3$ reduces the one-particle Hilbert space dimension for further identical quasielectrons by 5/3 (as compared to 0 for bosons or 1 for fermions). For quasiholes the corresponding diagonal exclusion coefficient is 1/3. However, there are also off-diagonal exclusion coefficients. For instance, an added quasielectron reduces the one-particle Hilbert space dimension for quasiholes by the coefficient $g+-$, and the corresponding coefficient $g-+$ is similarly defined.

In this work, the off-diagonal exclusion coefficients were extracted from exact numerical results for finite electron systems on a spherical surface. These coefficients were found, for quasielectrons (holes) near $\upsilon = 1/3$, to be +–5/3. This result is nontrivial, since the naive argument gives -+1/3, while the simple composite-fermion picture gives +–2/3. The corresponding coefficients (diagonal and off-diagonal) for quasiparticles near the general FQHE filling factor $\upsilon = p/(2np+1)$ were also obtained; and in each case, the diagonal coefficients agree with those obtained without correction from the composite-fermion picture, while the diagonal coefficients require systematic correction. Thus, it is clear that hard-core interactions among unlike quasiparticles must be responsible for the change in coefficients from these "naive" values.

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1. Summary of paper: *Phys. Rev. B* **55**, 6727 (1997).
2. University of Olso, Oslo, Norway.
3. Guest scientist from The University of Tennessee, Knoxville, Tenn.
4. University of Central Florida, Orlando, Fla.
5. M. D. Johnson and G. S. Canright, *Phys. Rev. B* **49**, 2947 (1994); G. S. Canright and M. D. Johnson, *J. Phys. A* **27**, 3579 (1994).

HIGH-TEMPERATURE SERIES EXPANSION FOR THE EXTENDED HUBBARD MODEL[1]

M. Bartkowiak,[2] J. A. Henderson,[3] J. Oitmaa,[4] and P. E. deBrito[5]

The Hubbard model plays the role of a standard model for correlated fermions on a lattice. In order to study commensurate sublattice charge ordering in narrow-band materials, the Hubbard model was extended to include an intersite electron-electron interaction. This model has subsequently been found to be of relevance also to high-temperature superconductors.

The high-temperature series expansion (HTSE) method has been used successfully to study systems of localized spins, providing excellent results for their critical properties. The structure of the Hubbard model and its extension are quite similar to the structure of the standard models in the theory of spin systems (e.g., Ising and Heisenberg models). Thus, one expects that HTSE should yield reliable information on the properties of these models for strongly correlated electron systems.

The single-band Hubbard model, extended by an intersite interaction, W, was studied. High-temperature series to the sixth order are obtained for the grand canonical potential, staggered magnetic susceptibility, charge-ordered susceptibility, and compressibility. These series are derived with general values of W and the intrasite interaction U for half-filling ($n = 1$) on a simple cubic lattice. It was found that the antiferromagnetic phase is stabilized by repulsive W, in the limit of strong intrasite repulsion. The effect of nonzero hopping t on the charge-ordered and condensed phases is also examined. It was also found that the critical temperature for transition to a condensed phase is reduced, while the charge-ordered phase is destabilized by t for small, positive or negative U and stabilized for large, negative U.

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1. Summary of papers: *Phys. Rev. B* **51**, 14077 (1995); *Mol. Phys. Rep.* **11**, 133 (1995).
2. ORNL/ORISE postdoctoral research associate.
3. Universitetet i Trondheim, Trondheim, Norway.
4. University of New South Wales, Kensington, Australia.
5. Universidade de Brasilia, Brasilia, Brazil.

LINKED CLUSTER EXPANSION AND 1/d EXPANSIONS FOR CLASSICAL SPIN SYSTEMS[1]

E. Halvorsen[2] and M. Bartkowiak[3]

The molecular field approximation (MFA) for classical spin systems becomes exact in the limit of infinite dimensionality d of the lattice. The first attempts to formulate an expansion in terms of the inverse powers of d for these systems were made more than 30 years ago. A great interest in the limit of infinite dimensions for correlated fermion systems has also arisen within the last few years, but the problem of interacting fermions in infinite dimensions is far more complicated than the MFA for classical spin models. Since the linked cluster expansion (LCE) with vertex renormalization for classical spin systems is quite analogous to propagator renormalized expansions for lattice fermions, it is beneficial to use classical spin models as a testing ground for $1/d$ expansions based on resummation of graphs. In addition, because some quantum models have a classical spin or a lattice gas model as a limiting case, $1/d$ expansions for the classical models can serve as benchmarks for other approximation schemes to the quantum models. Furthermore, perturbation expansions for correlated electron systems with the atomic limit as the unperturbed Hamiltonian are closely parallel to the LCE for classical spin systems.

Here, $1/d$ expansions for classical spin systems based on the vertex renormalized LCE were considered. The free multiplicities of the LCE graphs on a hypercubic lattice in an arbitrary dimension d are calculated using generating functions. The technique is applied to the Ising model and to a two-component classical lattice gas corresponding to an extended Hubbard model at half filling in the zero-bandwidth limit. A resummation of the LCE was used to generate $1/d$ expansions for the equation of state and for the critical temperature. The method, which is rather general and applicable to a wide range of models, proves convenient for calculating asymptotic power series expansions in $1/d$. The vertex renormalized expansion is shown to break down at low temperature in higher order approximations, barring attempts to construct simple approximations that are both self-consistent and exact to some finite order in $1/d$.

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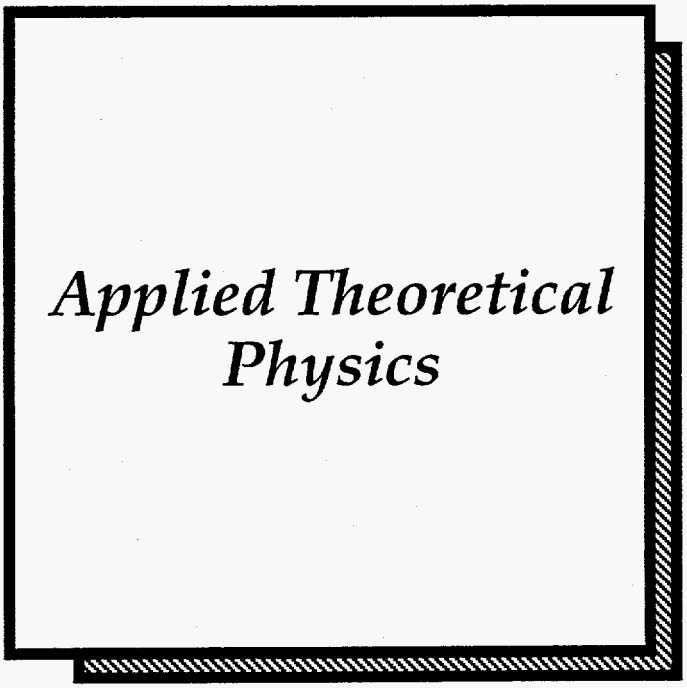
1. Summary of paper to be published.
2. Norwegian University of Science and Technology, Norway.
3. ORNL/ORISE postdoctoral research associate.


Applied Theoretical
Physics

DYNAMICS OF PLUME PROPAGATION AND SPLITTING DURING PULSED-LASER ABLATION[1]

R. F. Wood, K. R. Chen,[2] J. N. Leboeuf,[3] A. A. Puretzky,[4] and D. B. Geohegan

An innovative new approach has been developed for modeling the expansion of laser-generated plumes into low-pressure gases where initially the mean-free path may be long enough for interpenetration of the plume and background. The model is based on a combination of multiple elastic scattering and hydrodynamic formulations. Although relatively simple in structure, it gives excellent fits to new experimental data for Si in He and Ar and provides for the first time a detailed, coherent explanation of the observed splitting of the plume into a fast and slow component.

The plume is broken into orders corresponding to the number of collisions made with the background gas. The first order reaches the detector without any scattering, the second order undergoes one scattering event, etc. It is assumed that $\rho_\pi(t,x,k)$ is the density of the kth order plume at time t and distance x, ρ^s is the density scattered from $\rho_p(t,x,k)$, and $\rho_b(t,x,k)$ is the density of background gas. The total plume density $\rho_p(t,x,k)$ is a sum of $\rho_p(t,x,k)$ over k. At any time and in any spatial cell, collisions may occur which scatter particles from the k - 1 order into the kth order and from the kth order into the k + 1 order. While particles can only be transferred between the various orders by collisions, densities in the individual orders propagate to give the overall plume expansion. The propagation is determined by the usual equations for conservation of mass and momentum.

Figure 1 gives an overall comparison of the results for Si/Ar and Si/He when only head-on collisions are considered and the background gas is assigned an average velocity. It can be seen that the overall fits are excellent.

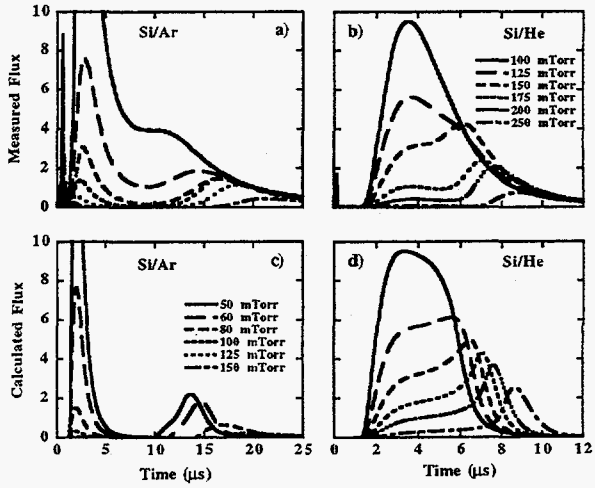


Fig. 1. Calculated and experimental flux results. Only the value of σ_{pb} was allowed to vary freely in going from He to Ar background gases. The fluxes have been normalized to a convenient scale for graphical presentation. One unit of flux on the graphs corresponds to 0.0125 A/cm^2 for Si9/AR and 0.125 A/cm^2 for Si/He.

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1. Summary of paper to be published.
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4. ORNL/ORISE postdoctoral research associate.

GROWTH AND DOPING OF Si LAYERS BY MOLECULAR-JET CHEMICAL VAPOR DEPOSITION: SOLAR CELL FABRICATION[1]

D. C. Lubben, G. Eres, G. E. Jellison, Jr., R. D. Westbrook,[2] and R. F. Wood

Chemical vapor deposition (CVD) of epitaxial Si is generally carried out at temperatures between 950° and 1200°C. These temperatures can lead to the redistribution of dopant atoms within the film as well as out-diffusion of substrate impurities into the deposited film. Several techniques have been employed to reduce the thermal load during growth, including rapid-thermal processing CVD (RTPCVD) and plasma-enhanced CVD (PECVD). In PECVD, deposition rates of several μm/hr at substrate temperatures as low as 750°C have been obtained.

Molecular-jet CVD (MJCVD) is another technique which can potentially produce epitaxial films at even lower temperatures and higher deposition rates. In MJCVD, a high-velocity gas jet, generated by a high-pressure expansion through a small nozzle, is used to deliver the source gas to a heated substrate. Molecular jets provide unique conditions not attainable with equilibrium growth methods. For example, the fluxes and incident kinetic energies of the species can be independently varied so that high deposition rates can be obtained at relatively low T_s.

The simultaneous growth and in situ doping of epitaxial Si films by MJCVD are studied in this work. Films were grown using a source gas of 10% Si_2H_6 in H_2 and were doped *p*- or *n*-type with B_2H_6 or PH_3, respectively. Some *p*-doped films were also grown by conventional very low pressure CVD (VLPCVD) for comparison. Films with *n*-type doping had a significant enhancement both in growth rate and dopant incorporation when deposited from the molecular jet. MJCVD was used to fabricate solar cells for the first time.

Figure 1 shows an I-V characteristic of one of the better cells. The short-circuit current, I_{sc}, is good while the open-circuit voltage, V_{oc}, and the fill factor, *FF*, are somewhat low compared with those in high efficiency cells.

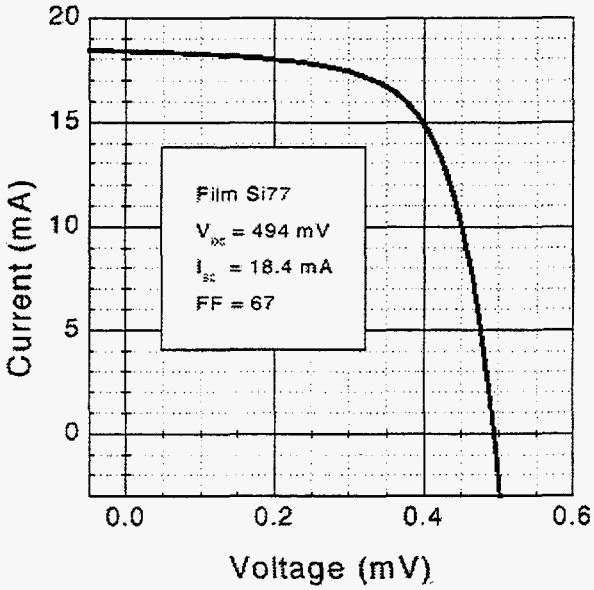

Fig. 1. I-V characteristics of an MJCVD solar cell.

1. Summary of paper to be published.
2. Consultant representing self.

FAILURE MODES AND ENERGY ABSORPTION CAPABILITY OF ZnO VARISTORS[1]

M. Bartkowiak,[2] G. D. Mahan,[3] and M. G. Combe[4]

Thermal and mechanical behavior of high-power ZnO surge arresters under current pulses of various magnitude and duration is simulated. By solving heat transfer equations for a varistor disk with nonuniform electrical properties, the time dependence of the temperature profile and the distribution of thermal stresses have been computed. This simple theoretical model can identify the energy handling limitations of ZnO varistors imposed by three different failure modes: puncture, thermal runaway, and cracking. Each failure mode can be limiting, depending on the disk shape, its electrical uniformity, and the current magnitude. The model conforms to the available failure data and explains the observation that energy handling improves at high current densities.

Cracking and puncture are caused by a localization of the current, which causes local heating leading to nonuniform thermal expansion and thermal stresses. Puncture is most likely in varistor disks with low geometrical aspect ratio and when the current density has intermediate values. Cracking dominates at higher current densities and for disks with a high aspect ratio. Puncture and cracking do not occur when the current is small, because the time evolution of the nonuniform heating is slow enough for the temperature distribution to flatten. They are also unlikely at very large currents corresponding to the upturn region of the I-V characteristic, because in this case the current becomes uniformly distributed. For low and very high current densities, the most likely failure mode is thermal runaway.

The model is also applied to evaluate the influence of the nonuniformity of varistor disks used in surge arresters on their energy handling capability. Puncture is the dominating failure mode for slightly nonuniform disks, but cracking becomes more likely as the degree of nonuniformities increases. It is shown that it is possible to minimize the chance of a failure of varistor disks at high-current pulses by adjusting their resistivity in the upturn region of the I-V characteristic.

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1. Summary of papers: *J. Appl. Phys.* **79**, 8629 (1996) and *IEEE Transactions Power Delivery* (in press).
2. ORNL/ORISE postdoctoral research associate.
3. UT/ORNL Distinguished Scientist.
4. Hubbell Power Systems, Centralia, Mo.

NONLINEAR CURRENTS IN ZnO VARISTORS[1]

M. Bartkowiak,[2] G. D. Mahan,[3] F. A. Modine, M. A. Alim,[3] R. Lauf,[4] and A. McMillan[4]

Zinc oxide varistors are multicomponent ceramic semiconductor devices with highly nonlinear current-voltage (I-V) characteristics. They are produced by sintering ZnO powder together with small amounts of other oxide additives. Because of the excellent nonlinear electrical properties (empirically $I = k\,V^{\alpha}$, where α can be 60 or higher at the breakdown) and very high current and energy absorption capabilities, ZnO varistors are widely used as electrical surge arresters. The nonohmic behavior of ZnO varistors is contributed by the grain boundaries. The varistor additives cause formation of double Schottky barriers at the grain boundaries, and the extreme electrical nonlinearity results from minority carrier creation in the grain boundary region that leads to breakdown of the barriers. However, a real varistor of macroscopic size is a complex multijunction device composed of a large number of various nonlinear and ohmic elements distributed in an irregular network and connected in parallel and in series.[5] Therefore, it is crucial to understand the relationship between the properties of the individual grain microjunctions and the global behavior of the random electrical networks which form polycrystalline varistor samples.

The first realistic model of transport properties of zinc oxide ceramic varistors has been constructed from two-dimensional Voronoi networks and studied via computer simulations. The model yields lucid explanations for several features of the current-voltage characteristics of zinc oxide varistors. These features, which are experimentally verified, include various shapes of the electrical characteristics; the difference between the average breakdown voltage per grain boundary and the breakdown voltage, which is measured directly across a grain boundary; and reduction of the nonlinearity coefficient of bulk varistors relative to that of isolated grain boundaries. The simulations clarify the problem of the influence of different types of electrical microjunctions at grain boundaries on the breakdown voltage and on the electrical nonlinearity of bulk varistor materials. It has been discovered that in the breakdown region polycrystalline varistors with nonuniform grain structure conduct the current almost exclusively through very narrow channels (paths). This current localization effect has important practical consequences for the energy handling capability of ZnO varistors.

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1. Summary of paper: *Phys. Rev. B* **51**, 10825 (1995).
2. ORNL/ORISE postdoctoral research associate.
3. Ohio Brass Company, Wadsworth, Ohio.
4. Metals and Ceramics Division, ORNL.
5. M. Bartkowiak et al., *J. Appl. Phys.* **80**, 6516 (1996).

NONUNIFORM HEATING IN ZINC OXIDE VARISTORS STUDIED BY INFRARED IMAGING AND COMPUTER SIMULATION

H. Wang,[1] M. Bartkowiak,[2] F. A. Modine, R. B. Dinwiddie,[3] L. A. Boatner, and G. D. Mahan[4]

ZnO varistors have highly nonlinear electrical characteristics and are widely used as devices for over-voltage protection. While varistors have a large capacity to absorb energy, they are, in fact, subject to occasional failure. The significant varistor-failure mechanisms include: electrical puncture, thermal cracking, and thermal runaway—all resulting from excessive heating, in particular, from nonuniform heating. Nonuniform heating of ZnO varistors by electrical pulses occurs on three different spatial scales: (1) microscopic (sub-micron), (2) intermediate (submillimeter), and (3) macroscopic (of the order of millimeters or centimeters). Heating on these scales has different origins and different consequences for device failure in large and small varistors.

On the microscopic scale, the heating in thin (e.g., 100-μm-thick) varistor slices is observed to be localized in strings of tiny hot spots. The hot spots occur at the grain boundaries in a conducting path where the potential is dropped across Schottky-type barriers and the heat is generated. These observations are interpreted by applying transport theory and using computer simulations. It is shown that the heat transfer on a scale of the grain size is too fast to permit temperature differences that could cause a varistor failure.

On an intermediate-size scale, the heating in small (e.g., 10-mm-diam and 1-mm-thick) varistor disks is most intense along localized electrical paths. The high electrical conductivity of these paths has microstructural origin (i.e., it derives from the statistical fluctuations in properties). It is found that influence of this statistical disorder changes with varistor size in a manner that can be described with relatively simple mathematics. Current localization on the intermediate-size scale appears to be significant only in small varistors.

On the macroscopic scale, heating in large (e.g., 42-mm-diam and 42-mm-thick) varistor blocks is usually greatest near the block edges and is approximately radial symmetric in blocks fabricated at a low aspect ratio. In blocks fabricated at a higher aspect ratio, the heating is less symmetric. Current localization in large blocks can be attributed to inhomogeneities in the electrical properties which originate during ceramic processing (e.g., compaction and sintering). Destructive failures (puncture and cracking) of large varistor blocks are shown to be caused by this nonuniform heating on a macroscopic scale.

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THE BEST THERMOELECTRIC[1]

G. D. Mahan[2] and J. O. Sofo[3]

Thermoelectrics are solid state materials which have high values of the Seebeck coefficient and electrical conductivity and small values of the thermal conductivity. Such materials can be used to make solid state refrigeration and solid state power generation devices. There is a continual search for materials which have these three characteristics.

This investigation answered the following questions: what features enable a material to be the best thermoelectric? Because the Seebeck coefficient and electrical conductivity are both properties of the conduction electrons in the solid, the discussion then focused on the question of what are the most desirable electronic properties. Given that one could arrange to have any density of states for the electron, or any lifetime, what would be the choice? A theorem was provided which proved that the best thermoelectric had a very singular feature in the effective density of states. This feature was at an energy value very close to the chemical potential. Whether this feature could be realized in an actual solid is a subject of great debate. The closest realization is to have a solid with rare-earth atoms, whose energy for the *f*-electrons is very near to the chemical potential. Such materials show high values of the Seebeck coefficient and electrical conductivity.

An additional theorem which put an upper bound on the figure of merit for thermoelectrics was proved. This bound is the most rigorous one every derived.

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1. Summary of paper: *Proc. Natl. Acad. Sci.* 97, 7436 (1996).
2. UT/ORNL Distinguished Scientist.
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Chapter 2

Neutron Scattering

Crystal Structure and Dynamics

MAGNETIC DYNAMICS IN UNDERDOPED $YBa_2Cu_3O_{7-x}$[1]

P. Dai, M. Yethiraj, H. A. Mook, T. B. Lindemer,[2] and F. Dogan[3]

Since the discovery of high-temperature cuprate superconductors in 1986, there has been a worldwide race to study these fascinating materials that are distinctly different from previously known superconductors. Above the superconducting transition temperature T_c, these materials display unusual normal state properties that suggest the opening of a pseudogap (a suppression of spectral weight) in the spin- or charge-excitation spectrum. The central issue is whether the physics of underdoped cuprates is fundamentally different from the description of the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity. Although recent photoemission and nuclear magnetic resonance (NMR) experiments suggest the opening of the pseudogap above T_c in underdoped cuprates, no one has established its correlation with the eventual superconductivity. Magnetic inelastic neutron scattering is a powerful bulk probe which gives direct information about the electrons in materials. This information is particularly important for high-temperature superconductors because they provide constraints on a possible microscopic theory for high-T_c superconductivity. A previous polarized neutron scattering experiment by Mook et al.[4] has established that the low-temperature magnetic excitation of optimally doped $YBa_2Cu_3O_{7-x}$ (YBCO) is dominated by a resonance that is sharp in energy, located at 41 meV, and centered at (π,π) in the reciprocal lattice. Subsequent measurements have shown that superconductivity opens a gap in the spin fluctuation spectra for these optimally doped YBCO superconductors. To study the evolution of the magnetic excitation as a function of oxygen doping, the first polarized neutron scattering measurements were made on an underdoped YBCO ($x = 0.4$). Results[1] show that the low-temperature spin excitations in the superconducting state for underdoped compounds are essentially the same as for the fully doped materials except for a change in energy scale. The unusual resonance, found at 41 meV in the fully doped materials, is moved to 34.8 meV for the underdoped $YBCO_{6.6}$. Furthermore, the enhancement at the resonance is accompanied by a suppression of magnetic fluctuations at both higher and lower energies.

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1. Summary of paper: *Phys. Rev. Lett.* 77, 5425 (1996).
2. ORNL retiree.
3. University of Washington, Seattle, Wash.
4. H. A. Mook et al., *Phys. Rev. Lett.* 70, 3490 (1993).

CRYSTAL CHEMISTRY OF $HgBa_2Ca_{n-1}Cu_nO_{2n+2+\delta}$ (n = 1, 2, 3, 4) SUPERCONDUCTORS[1]

M. Paranthaman[2] and B. C. Chakoumakos

Constant wavelength neutron powder diffraction data at room temperature were used to refine the crystal structures of $HgBa_2Ca_{n-1}Cu_nO_{2n+2+d}$ (n = 1, 2, 3, 4) superconductors, which were synthesized by solid state reaction of the component oxides. Samples annealed in both oxygen and argon atmospheres were examined. Rietveld refinements converged to values of R_{wp} = 8–10% and χ^2 = 1.1–1.7 using a tetragonal cell with P4/mmm symmetry. The $HgBa_2CuO_{4+d}$, $HgBa_2CaCu_2O_{6+\delta}$, and $HgBa_2Ca_2Cu_3O_{8+\delta}$ (n = 1, 2, and 3) samples were nearly single phase, whereas the $HgBa_2Ca_3Cu_4O_{10+\delta}$ (n = 4) sample was primarily a mixture of the n = 3 and 4 phases. For increasing n, the oxygen-annealed samples exhibit T_c (diamagnetic onsets) of 94, 123, 134, and 124 K, respectively, and a contraction of the CuO_2 sheets (lattice parameter "a"). The highest T_c sample, $HgBa_2Ca_2Cu_3O_{8+\delta}$, has the shortest apical Cu-O bond. Consistently, the atomic displacement parameter for Hg is large. The oxygen site within the Hg layer is partially occupied, and its occupation increases with increasing n. For the argon-annealed samples, the cell volume increases slightly because of the isotropic increase of both the cell parameters and T_c decreases. For $HgBa_2CaCu_2O_{6+\delta}$, the occupancy of the oxygen site within the Hg layer decreases upon annealing in argon, yet the T_c increased, implying that the initial carrier concentration is in the overdoped regime.

That the Hg cuprate family is similar structurally to other polysomatic series of cuprate superconductors is evident if the layer-stacking repeat for the primitive cell minus that of the respective n = 1 member is plotted vs. the mole % $CaCuO_2$ for five series. The thickness of the "infinite-layer"-type $CaCuO_2$ closely matches the $CaCuO_2$ layer module thickness derived from these polysomatic series, and the n > 1 members simply contain additions of exact multiples of this layer module. This perspective suggests that the thickness of the charge reservoir blocks is a key feature to correlate with the intrinsic behavior of the magnetic irreversibility field among the different series. Although the magnetic irreversibility field behavior tends to be dominated by the microstructure of the material, for materials with similar microstructures, the smaller the spacing of the reservoir blocks, the weaker is the temperature dependence of the irreversibility field. For example, comparing the same n-member, the intrinsic irreversibility field should improve in the series two-layer BiO cuprate < two-layer TlO cuprate < single-layer TlO cuprate < Hg cuprate < TlPb cuprate.

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1. Summary of paper: *J. Solid State Chem.* **122**, 221 (1996).
2. Analytical and Chemical Sciences Division, ORNL.

SURFACE AND BULK LATTICE DYNAMICS OF PEROVSKITES

J. Zhang,[1] P. Dai, E. W. Plummer,[2] H. A. Mook, P. A. Dowben,[3] and S. H. Liou[3]

One of the most important issues associated with the coupled electronic and magnetic phase transitions in "colossal magnetoresistance" (CMR) materials ($La_{1-x}A_xMnO_3$, A = Ca, Sr, Ba) is the static and dynamic lattice distortions accompanying the transitions. With neutron and electron scattering, both the bulk and surface lattice properties across the Curie temperature (T_c) of $La_{1-x}Ca_xMnO_3$ (x = 0.1 and 0.35) have been studied. Neutron diffraction results show a dramatic Ca-doping dependence of the lattice distortion anomaly at T_c (Fig. 1).[4] It was found that a static lattice distortion anomaly at T_c is associated with the magnetic phase transition and a dynamic lattice distortion anomaly at T_c is coupled to the metal-to-nonmetal transition. These results clearly indicate that both the static and dynamic Jahn-Teller-type lattice distortions play a crucial role in the bulk CMR materials. Electron scattering results, however, show that the surface lattice dynamics are quite different from the bulk.[5] The surface optical phonons have higher energy than the bulk modes, though the temperature dependence of phonon energies is similar to that of the bulk ones. A 2–4-meV shift in phonon energy across T_c is associated with a static lattice distortion related to the magnetic phase transition. The small energy dispersion and large linewidth of the surface phonons reflect the localized dynamic behavior. The different lattice dynamics at the surface are associated with the surface effects, including both the inherent reduction in symmetry and the preferential segregation of Ca to the surface. With angle-resolved x-ray photoelectron spectroscopy, a strong Ca surface segregation and a doping dependence of surface termination in the thin films of these CMR materials were found.[5]

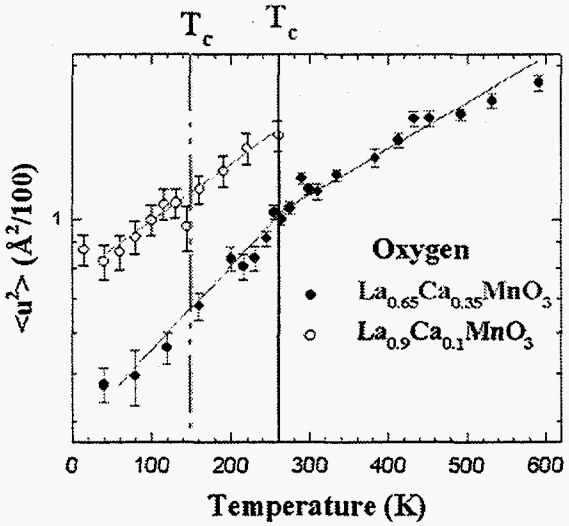

Fig. 1. Isotropic Debye-Waller factors of oxygen as a function of temperature. The Curie temperatures are clearly marked. Solid lines are guides for the eye.

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2. ORNL/UT Distinguished Scientist.
3. University of Nebraska-Lincoln, Lincoln, Nebr.
4. P. Dai et al., *Phys. Rev. B* **54**, R3694 (1996); *Solid State Commun.* **100**, 865 (1996).
5. J. Zhang and E. W. Plummer, *Surface Science*, to be published; J. Choi et al., *Physical Review B*, to be published.

STRUCTURAL AND MAGNETIC PROPERTIES OF $La_{0.5}Ca_{0.5}MnO_3$[1]

J. A. Fernandez-Baca, P. Dai, B. C. Chakoumakos, J. W. Cable,[2] S. E. Nagler, P. Schiffer,[3] N. Kalechofsky,[2] M. Roy,[2] Y.-K. Tsui,[3] P. l. J. McGinn,[3] S. L. Einloth,[3] and A. P. Ramirez[4]

There is a current interest in understanding the unusual magnetic and transport properties of the perovskite-based manganite compounds of the form $A_{1-x}B_xMnO_3$ (A = La, Pr, Nd; B = Ca, Sr, Ba). The most studied materials have been those with $x \approx 1/3$, which typically exhibit "colossal" magnetoresistance associated with a transition from a high-temperature paramagnetic insulator to a low-temperature ferromagnetically ordered metal. For other doping concentrations, the low-temperature phases exhibit a rich variety of behaviors, including ordinary and canted antiferromagnetism (AF), ferromagnetism (FM), and the spin-glass state. A particularly interesting limit arises for $x = 1/2$, for which the low-temperature structure is generally a charge-ordered state. The magnetic structures of the whole manganite series were studied experimentally and theoretically about 40 years ago,[5] but in spite of these early investigations, many features of the ordered state of the $x = 1/2$ compound are still unknown. The paramagnetic phase is separated from the low-temperature AF CE state by an intermediate FM phase, and recently the existence of incommensurate charge ordering in this intermediate phase has been reported. To address these issues, neutron diffraction, resistivity, and magnetization measurements were performed on $La_{1-x}Ca_xMnO_3$ with $x \approx 0.5$. These results indicate that the low-temperature magnetic structure of this compound is of a pseudo-CE-type in which the components of the spins in the a-c plane exhibit CE (AF) ordering while there is a net FM component along the b-axis. In the intermediate FM phase, it was found that there was charge ordering associated with AF short-range order. No evidence that would support the existence of a purely charge-ordered FM has been found.

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1. Summary of paper to be published.
2. ORNL retiree.
3. University of Notre Dame, Notre Dame, Ind.
4. Bell Laboratories, Lucent Technologies, Murray Hill, N.J.
5. E. O. Wollan and W. C. Koehler, *Phys. Rev.* **100**, 545 (1955); J. B. Goodenough, *ibid.*, 564 (1955).

NOVEL FERROMAGNETISM IN $SrRuO_3$

S. E. Nagler and B. C. Chakoumakos

$SrRuO_3$ is a ceramic metal with a slightly distorted cubic perovskite structure. It is a prime example of the class of materials termed as extended electron compounds—compounds whose electronic properties are dominated by transition-metal atoms in the 4*d* and 5*d* series of the periodic table.

$SrRuO_3$ is closely related to the unusual proposed triplet superconductor Sr_2RuO_2. $SrRuO_3$ becomes ferromagnetic below T_c = 160 K. The magnetism arises primarily from the 4*d* Ru atoms, but because of the extended nature of the electrons, hybridization with oxygen *p* orbitals is also very important. Polarized neutron scattering measurements in $SrRuO_3$ have been made, and it has been shown directly that approximately 10% of the magnetic moment is carried by the oxygen atoms. This is the first example of a ferromagnetic metal with oxygen moments.

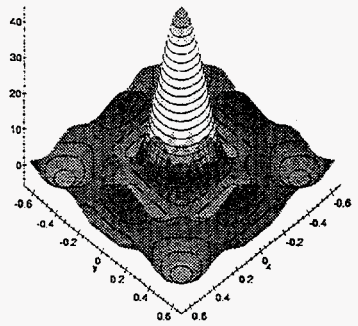

Fig. 1. Magnetization density in $SrRuO_3$ determined from polarized neutron diffraction. The density plotted is from the central plane of a pseudo-cubic unit cell. The large peak in the center arises from the Ru atom and the four smaller peaks are the surrounding oxygen atoms.

QUANTUM SPIN DIMERS[1]

S. E. Nagler, D. A. Tennant,[2] F. E. Barnes,[3] A. W. Garrett,[4] and C. C. Torardi[5]

Spin dimers are perhaps the simplest interacting quantum systems. They are ideal model systems for studying the superexchange interactions that are central to solid state magnetism. A particularly interesting example consisting of pairs of $S = 1/2$ V^{4+} ions in the material $VODPO_4 \bullet 1/2D_2O$ (VODPO) has been examined. Using inelastic neutron scattering, it has been shown that the spins constituting the dimer pairs in VODPO have been misidentified in the research literature. The correct dimer pairs consist of V^{4+} ions interacting through a covalently bonded PO_4^{3-} complex. This result casts doubt on the identification of the related material $VO_2P_2O_7$ as a spin ladder. It also illustrates the fact that covalent complexes should afford excellent opportunities for creating novel magnetic structures and engineering exchange strengths in magnetic materials.

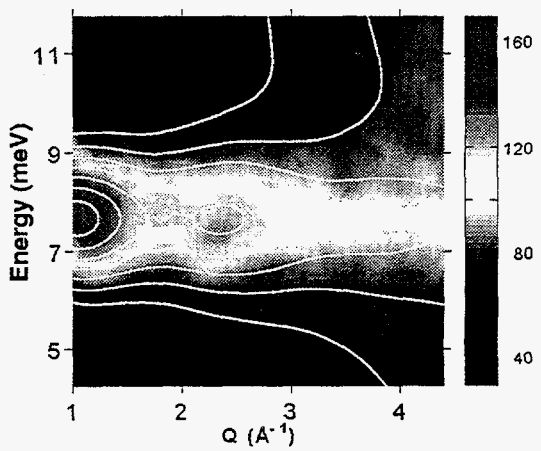

Fig. 1. Neutron scattering in VODPO. Intensity is represented by shading. Control lines illustrate a fit to a spin dimer model. The peak positions allow the dimer to be identified.

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1. Summary of paper: *Physical Review Letters* (in press).
2. ORNL/ORISE postdoctoral research associate.
3. Physics Division, ORNL, and The University of Tennessee, Knoxville, Tenn.
4. Graduate student from the University of Florida, Gainesville, Fla.
5. Dupont Research, Wilmington, Del.

MAGNETIC EXCITATIONS IN THE ALTERNATING CHAIN VOPO[1]

S. E. Nagler, D. A. Tennant,[2] B. C. Sales, F. E. Barnes,[3] and A. W. Garrett[4]

The material $VO_2P_2O_7$ (VOPO) has long been considered as the prototypical example of a two-leg $S = 1/2$ antiferromagnetic Heisenberg spin ladder. There has been intense interest in spin ladders recently because of the realization that they may be present in and important for high-T_c superconductors and the prediction that doped ladders may also superconduct. Inelastic neutron scattering experiments have been performed on VOPO using both powders and more recently an array composed of approximately 200 single crystals. Measurements on VOPO single crystals have determined the dispersion relations for magnetic excitations which directly reflect the spin Hamiltonian. The results show that VOPO is actually an example of an alternating chain system and that the existing research literature on VOPO as a spin ladder is in fact wrong. Further, investigations have revealed that a novel triplet two-magnon bound state is present in alternating chains. Our work sheds new light on the physics of low-dimensional quantum systems.

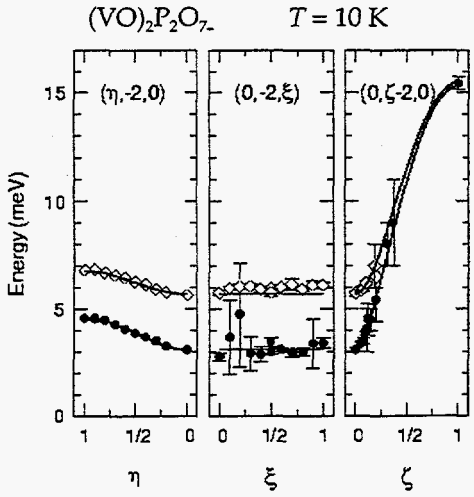

Fig. 1. Dispersion relations of spin-wave excitations in VOPO.

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1. Summary of paper: *Physical Review Letters* (in press).
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MAGNETIC ION-LATTICE INTERACTIONS IN $YbPO_4$[1]

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Interactions of rare-earth (RE) ions with their host lattice have previously been the subject of a number of spectroscopic investigations. Among the various systems that one might consider, the RE orthophosphate series, $REPO_4$ (*RE* = Tb to Lu), is ideally suited to a systematic study of RE-host-lattice interactions because these materials have a relatively simple body-centered-tetragonal crystal structure of the zircon-type (space group $I4_1/amd$). In this structure, all the RE atomic sites exhibit one equivalent unique point-group symmetry. In these insulating compounds, crystal-field (CF) transitions between low-lying states of the RE ions and atomic vibrations (phonons) are the primary excitations responsible for a number of important thermodynamic and magnetic properties at low temperatures.

Strong CF-phonon interactions may be manifested in anomalous properties, including magnetoelastic effects and Jahn-Teller-type transitions. The first unambiguous indications of a strong CF-phonon coupling in $YbPO_4$ was provided by Raman and Brillouin scattering studies.[6] Subsequently, Nipko and coworkers[7] have observed an anomalous softening of the C_{11}–C_{12} elastic constants of $YbPO_4$ at low temperatures by means of Brillouin scattering, and this result suggests that a Jahn-Teller-type coupling occurs between the low-lying electronic states of the Yb^{3+} ions and the B_{1g} lattice-strain mode—even though a cooperative structural phase transition does not take place.

In the present investigations, the magnetic phonon excitation spectra of $Yb_xLu_{1-x}PO_4$ (x = 0, 0.25, and 1) were measured using inelastic neutron scattering, in order to examine the strength of CF-lattice coupling as a function of the Yb-ion concentration. Excitations from the ground state to the three upper CF-split states of the Yb^{3+} $^2F_{7/2}$ multiplet were identified, but the peaks are anomalously broad. Additionally, the phonon density of states of $YbPO_4$ shows broadened phonon bands in the range 10–60 meV. The results provide evidence for the existence of strong CF-phonon interactions within the Brillouin zone.

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1. Summary of paper: *Journal of Physics: Condensed Matter* (in press).
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3. Technische Universität Dresden, Dresden, Germany.
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6. P. C. Becker et al., *Phys. Rev. B* **45**, 5027 (1992).
7. J. Nipko et al., *Phys. Rev. B* **53**, 2286 (1996).

CRYSTAL-FIELD SPLITTING AND ANOMALOUS THERMAL EXPANSION IN $YbVO_4$[1]

J. C. Nipko,[2] C.-K. Loong[2], S. Kerr,[3] M. M. Abraham,[4] and L. A. Boatner

Motivated by their importance in diverse areas such as laser/phosphor host media and Jahn-Teller-type phase transitions, a systematic study of the 4f-electron crystal-field-level structure in the rare-earth (RE) orthophosphate and RE orthovanadate compounds has been initiated by means of neutron spectroscopy and magnetic-susceptibility measurements.[5,6]

In the present work, a study of the crystal-field effects and thermal expansion in the specific case of $YbVO_4$ has been carried out using neutron scattering. Evidence for three magnetic transitions was established from the scattering function obtained from a polycrystalline sample of $YbVO_4$.

The temperature dependence of the **a** and **c** lattice parameters of the tetragonal unit cell was determined by neutron diffraction, and at low temperatures, the **c** lattice parameter of $YbVO_4$ exhibits a minimum at ~120 K, while the **a** lattice parameter decreases much more rapidly with temperature than the corresponding parameter in $LuVO_4$. Using the crystal-field wave functions obtained from the crystal-field model, the quadrupole moment of the Yb^{3+} ions in $YbVO_4$ was calculated as a function of temperature. The calculations show a behavior similar to the anomalous temperature dependence of the lattice parameters. No such anomalies are observed when Yb^{3+} is replaced with Lu^{3+} (which shows no 4f magnetism) in these materials. These observations strongly suggest that the anomalies in the temperature dependence of the lattice parameters arise from a RE quadrupolar interaction with the crystalline lattice. In principle, RE quadrupole-moment lattice couplings of this type will also affect other physical properties of this system.

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1. Summary of paper: *Journal of Alloys and Compounds* (in press).
2. Argonne National Laboratory, Argonne, Ill.
3. Colorado State University, Fort Collins, Co.
4. ORNL retiree.
5. C.-K. Loong et al., *J. Chem. Phys.* **98**, 4214 (1993).
6. C.-K. Loong et al., *J. Phys. C: Condensed Matter* **5**, 5121 (1993).

NEUTRON DIFFRACTION AND PHASE EVOLUTION OF MECHANICALLY ALLOYED ζ-$FeZn_{13}$ INTERMETALLIC PHASES[1]

O. N. C. Uwakweh,[1] J. Liu,[2] A. Jordan,[2] B. C. Chakoumakos, S. Spooner, and P. J. Maziasz[3]

Mechanical alloying of elemental constituents for the purpose of forming or synthesizing intermetallic phases is well established as a valid means of generating unanticipated materials properties. In the case of Fe-Zn phases, the large difference between the melting points of Fe and Zn always leads to compositional changes arising from the high vapor pressure of Zn when traditional melting processes are used. The importance of the Fe-Zn intermetallic phases is due to their occurrence at the substrate-coating interface of galvanized iron. High-energy ball-milling with subsequent annealing is used to synthesize the intermetallic compound ζ-$FeZn_{13}$. The as-milled product is a mechanical mixture of Fe and Zn. Annealing at 350°C transforms the mixture to the stable intermetallic phase. Differential scanning calorimetry identifies two characteristic stages of the phase formation process with activation energies of 128 and 202 kJ/mole. The first stage begins at 218°C and is associated with short-range atomic diffusion enhanced by defect annihilation or elimination. The second stage occurs at 310°C and is associated with continued transformation involving both long-range diffusion and recrystallization. Rietveld refinement of neutron powder diffraction data for the stable phase confirm the C2/*m* crystal structure of ζ-$FeZn_{13}$, a = 14.4099(3) Å, b = 7.6058(1) Å, c = 5.0762(1) Å, and β = 127.185(1)°. The crystal structure consists of icosahedral Zn clusters with Fe at their centers; these share corners along the *c*-direction and are closest-packed in the (001) plane, but this packing is distorted by additional Zn atoms (Fig. 1). At 565°C the ζ-$FeZn_{13}$ transforms to δ + liquid according to a peritectic reaction with a heat of 737 kJ/mole observed by calorimetry.

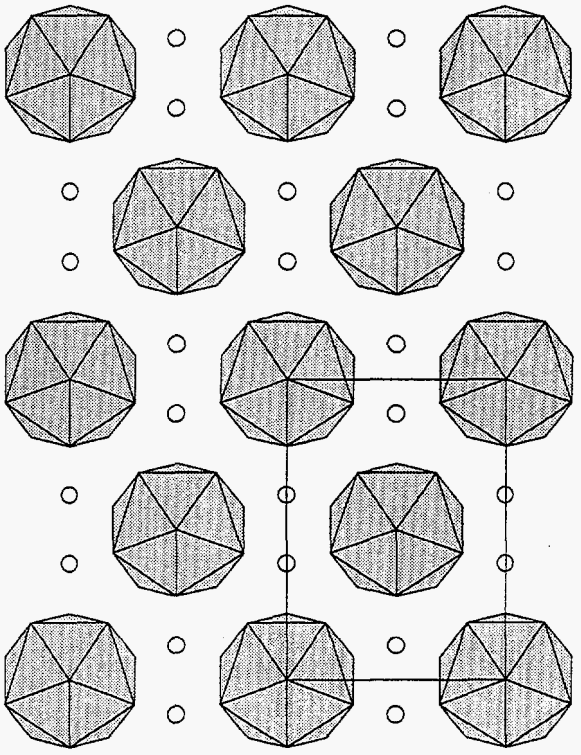

Fig. 1. Atomic arrangement of ζ-$FeZn_{13}$ showing the icosahedral Zn clusters (shaded) and additional Zn atoms (open circles). The unit cell is outlined, and the viewing direction is [001].

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1. Summary of paper: *Metallurgical and Materials Transactions* (in press).
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STRUCTURAL, MAGNETIC, AND TRANSPORT PROPERTIES OF $La_2Cu_{1-x}Li_xO_4$[1]

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J. D. Thompson,[3] B. C. Chakoumakos, and S. E. Nagler

Hole-doping mechanisms in the cuprate superconductors have been explored by various chemical substitutions. La_2CuO_4 is the archetype cuprate superconductor (Fig. 1), and a particularly interesting in-plane substitution is that of Li for Cu. Li^{1+} has an ionic radius essentially the same as that of Cu^{2+}, does not have a magnetic moment, and brings a hole with it to the plane. This hole appears to be localized; consequently, it is interesting to compare the effects of the in-plane substituted holes with the mobile holes introduced by out-of-plane substitutions. Li substitutes for Cu in La_2CuO_4 up to the limiting stoichiometry $La_2Cu_{0.5}Li_{0.5}O_4$, which exhibits a superstructure order. The effects of this in-plane hole doping on the structural and magnetic properties of La_2CuO_4 are very similar to those due to Sr for La substitution. The tetragonal-orthorhombic structural phase transition occurs for a given amount of Sr or Li at nearly the same temperature, and the in-plane lattice constant of $La_{2-y}Sr_yCu_{1-x}Li_xO_4$ at room temperature depends only on the combined hole count $(x + y)$ and not on the individual Sr or Li substitution. Long-range magnetic order is destroyed upon substitution of 3% Li for Cu, analogous to the effect of Sr for La substitution on T_{Neel}. In contrast, however, the holes introduced by Li substitution are bound, and the resistivity as a function of temperature is non-metallic for all Li concentrations.

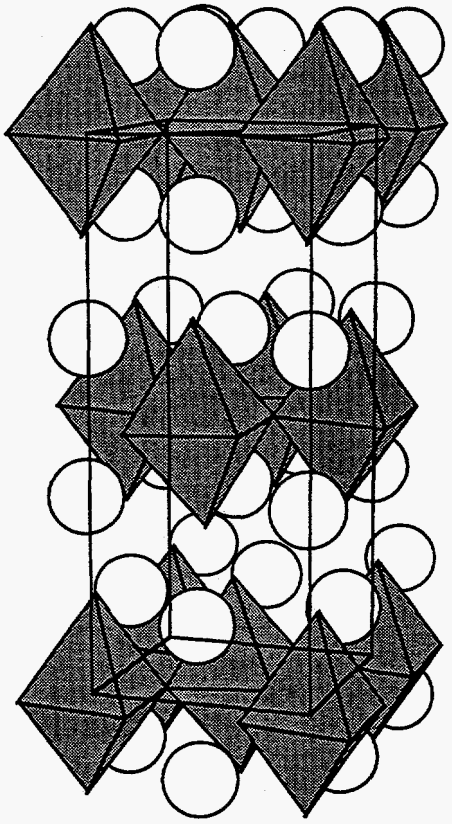

Fig. 1. Crystal structure cartoon for orthorhombic La_2CuO_4, where the CuO_6 units are shown by shaded polyhedra. The open circles represent the La atom positions.

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1. Summary of paper: *Physical Review B* (in press).
2. Florida State University, Tallahassee, Fla.
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NOVEL SYNTHESIS AND STRUCTURE REFINEMENTS OF $Li_4Mn_5O_{12}$ FOR RECHARGEABLE LITHIUM BATTERIES[1]

T. Takada,[2] E. Akiba,[2] F. Izumi,[3] and B. C. Chakoumakos

Lithium manganese oxides are potentially excellent cathode materials for advanced rechargeable lithium batteries because they offer high cell voltage, good rechargeability, a wide range of operating temperatures, and lower cost as compared with $LiNiO_2$ and $LiCoO_2$. For the Li-Mn-O family of spinel compounds (Fig. 1), the onset of structural changes caused by the Jahn-Teller distortion upon deep discharging could be suppressed by introducing a small amount of Li ions into the 16*d* sites to keep the average Mn oxidation state slightly above 3.5. The solid solution range in this spinel family is large, and the exact composition of the spinel electrode plays an important role in controlling the rechargeability. Understanding the crystal structural changes during the synthesis process is crucial for both process control and understanding the variation of the voltage, the capacity, and the cycling performance of spinel-based battery cells. Well-crystallized $Li_4Mn_5O_{12}$ powder was prepared by heating an eutectic mixture of lithium acetate and manganese nitrate in an oxygen atmosphere. The structure of $Li_4Mn_5O_{12}$ was found to be cubic spinel by Rietveld refinement of both neutron and x-ray powder diffraction data. The lithium ions occupy both the tetrahedral sites 8*a* and part of the manganese sites 16*d*, but not the 16*c* sites, and all the manganese ions occupy 16*d* sites. The lattice parameter was determined to be sensitive to the synthesis temperature, as a consequence of the variation in manganese valence. The presence of Mn^{3+} leads to the formation of a stoichiometric spinel $LiLi_xMn_{2-x}O_4$ in which x decreases from 1/3 ($Li_4Mn_5O_{12}$) to 0 ($LiMn_2O_4$), with concomitant formation of Li_2MnO_3 depending on the synthesis conditions.

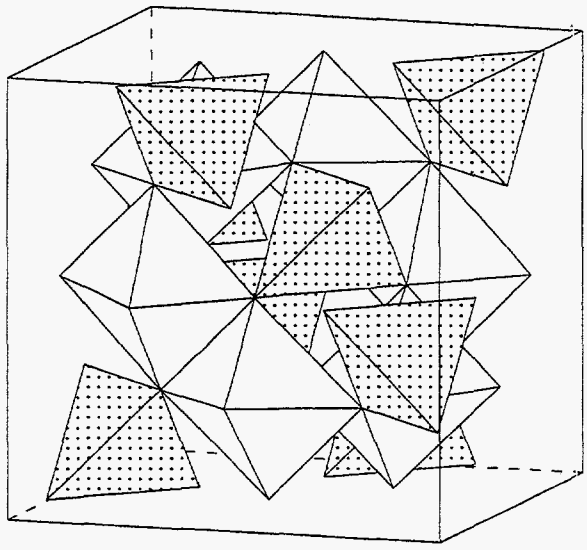

Fig. 1. Spinel structure showing the octahedral (16*d*) and tetrahedral (8*a*) sites as shaded polyhedra.

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1. Summary of papers: *J. Solid State Chem.* **130**, 74 (1997); *Journal of Power Sources* (in press).

2. National Institute of Materials and Chemical Research, Tsukuba, Ibaraki, Japan.

3. National Institute for Research in Inorganic Materials, Tsukuba, Ibaraki, Japan.

EFFECTS OF TRAVELING SURFACE ACOUSTIC WAVES ON NEUTRON BRAGG DIFFRACTION FROM PERFECT CRYSTALS

W. A. Hamilton and M. Yethiraj

The effect of bulk acoustic waves generated in single crystals on x-ray and neutron scattering has been studied for several decades now. More recently, there have been studies on the effects of surface acoustic wave (SAW) distortions on Bragg diffracted x-ray intensities. This work is the first investigation of the corresponding neutron case and, as such, of the Doppler effects consequent upon comparable velocities of the SAW and the Bragg-diffracted radiation.

Measurements were performed on the transit region of an interdigitated transducer SAW delay line configured on the surface of a perfect crystal of lithium niobate for the (030) reflection in symmetric Bragg geometry (Fig. 1). At an acoustic power of 200 mW, the amplitude of the 37-MHz SAW was about 15 Å over a 94-μm wavelength. This distortion has an effective mosaic ~60 μrad, about an order of magnitude greater than the reflection's Darwin plateau width, penetrating to a depth of ~1 acoustic wavelength.

Figure 2 shows the variation observed in the total diffracted intensity as the delay line was rotated about the scattering vector/surface normal for neutrons with transverse speeds slower, equal, and faster than the SAW. Slower neutrons showed significant enhancement of reflected intensity for all orientations, with a maximum when neutron beams and SAW move in opposite senses ($\phi = 180°$). Neutrons of equal traverse speed were also more strongly reflected at $\phi = 180°$, but the minimized sampling "pacing" of the distortion at $\phi = 0°$ gives no SAW enhancement. Surprisingly, for neutrons only a little faster than the SAW, the enhancement was negligible for all orientations. This observation contradicts our qualitative expectations from an analogy with a moving mosaic crystal. As yet, there is no quantitative theory for the interaction between the neutron and the coherent surface phonons in these measurements.

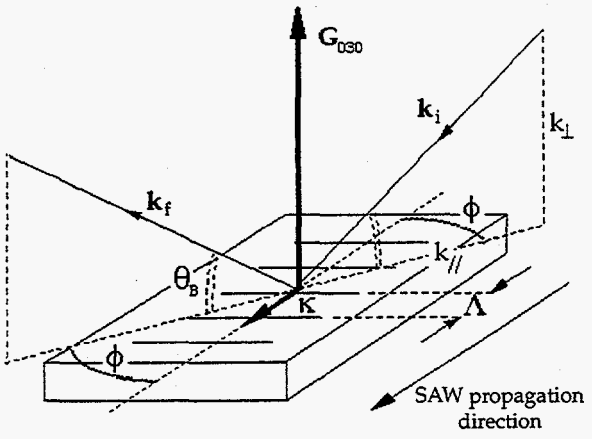

Fig. 1. The surface of a perfect crystal of LiNb for the (0.30) reflection in symmetric Bragg geometry.

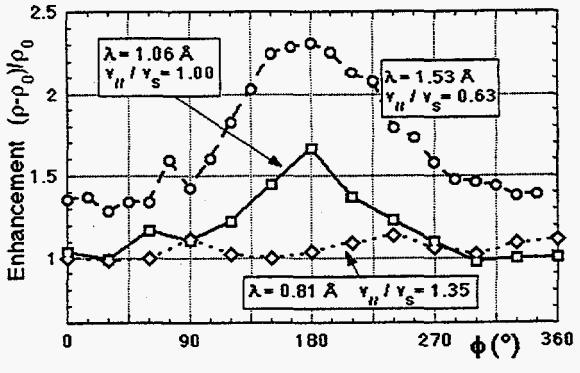

Fig. 2. Variation of diffracted intensity with rotation.

VERTICALLY FOCUSING Ge MONOCHROMATOR INSTALLED ON THE NEUTRON POWDER DIFFRACTOMETER

B. C. Chakoumakos, M. C. Wright,[1] G. B. Taylor, R. G. Maples, S. Spooner, and H. A. Mook

To deliver more neutron flux to the sample for Debye Scherrer powder diffraction, a vertically focusing monochromator (VFM) has been constructed using hot-pressed germanium crystals. A large, 7-cm-diam × 14-cm-long, single-crystal Ge boule was acquired from Tennelec/Nucleus, Inc., Oak Ridge, Tennessee. The boule ends were cut flat, and the crystal was hot-pressed several times to increase the crystal mosaic. Spatial mapping of the crystal mosaic by neutron diffraction suggested that the hot-pressing treatments had achieved some increase of the mosaic, but it was not completely uniform throughout the crystal. At this stage, the crystal was oriented using real-time x-ray Laue methods with calculated reference patterns generated by the LaueX software. In preparation for cutting, (100) and (0-11) reference flats were ground onto the crystal boule. After embedding the crystal in a glass-bead/epoxy matrix, the whole crystal was sliced at once into (511) slabs, 10-mm thick, using an industrial gang saw at Commercial Crystals, Inc., Naples, Florida. Next the (511) slabs were aligned and cut into (0-11) bars, 11-mm thick, using the same methods. During the cutting, each Ge crystal segment was coded so that spatial mapping of the crystal mosaic for individual segments could be used to reconstruct that for the whole crystal boule. The screening of crystal segments was initially done using the HB-1B neutron spectrometer which has a Ge crystal monochromator selecting a 1.1-Å wavelength. It was found that the hot-pressing was more effective on the exterior portions of the crystal boule, whereas the core region was less affected. Seven long segments with symmetric rocking curves and large mosaics were selected and mounted on a 15-element VFM mechanism designed and built by Techmod, Kailua, Hawaii. The crystal segments were held onto the VFM by clamping one end, and their orientation allows the (311), (511), and (711) reflections to be used by small rotations of the monochromator plug angle. Final adjustments of each crystal segment were done with the high-precision sample stage of the residual stress neutron spectrometer at HB-2. The motorized VFM was mounted eucentrically on a small motorized arc which was in turn mounted on a short motorized translation stage. This entire assembly is sufficiently compact that it was mounted on the inner plug of the HB-4 monochromator shield. Computer control of the focus, arc, translation, and plug angle was established. Qualitative appraisal of the VFM effect was made by recording a video of the incident beam using a neutron camera. A more quantitative appraisal shows as much as a threefold increase in intensity for small sample volumes.

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1. Instrumentation and Controls Division, ORNL.

THERMAL NEUTRON SCATTERING UPGRADES AT HFIR

J. L. Robertson

The facilities upgrade at HFIR includes significant improvements in the performance of beam-line instrumentation that utilizes thermal neutrons. The latest techniques are being used to design and optimize the neutron beam optics and source configuration for all thermal beams at HFIR. When completed, these beams will be the brightest available anywhere for neutron scattering.

The HB-2 beam tube has been completely redesigned so that it couples to a thermal guide system that will supply several instruments. The current project includes four instruments inside the confinement building with possible future expansion into a thermal guide hall. The complement of instruments involved includes a high-resolution powder diffractometer (existing), a wide-angle neutron diffractometer (WAND) (existing), a triple-axis spectrometer (new), and a residual stress instrument (new). The new design employs an innovative approach involving scatter wedges to maximize the performance of the thermal guide system. The guide system will accommodate up to five guides, three of which will be used for the four instruments above. These improvements to the thermal beam delivery system will increase the total number of neutrons available at the sample position by as much as a factor of 5.

The HB-1 and HB-3 beam tubes will be modified to accommodate larger beams so that the instruments supplied by them (primarily the HB-1, HB-1A, and HB-3 triple-axis spectrometers) can take greater advantage of focusing monochromators. The new shutters will have two apertures for beams at the triple-axis monochromator position. A 35-mm-wide by 150-mm-high beam will be used for high-resolution experiments, in conjunction with a vertically focusing monochromator. The second aperture will provide a 50-mm-wide by 120-mm-high beam to be used with a doubly focusing monochromator for experiments where flux is more important than high resolution. The upgrades will be completed in 2000 as part of the planned reflector replacement at HFIR.

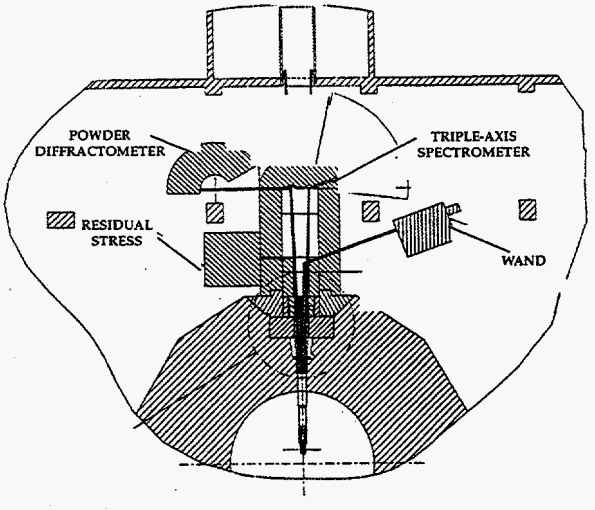

Fig. 1. Preliminary layout for neutron scattering instrumentation and guides at the HB-2 location at HFIR.

Large-Scale Structures

EFFECT OF QUARTZ SURFACE ON BULK SOLUTION STRUCTURES UNDER FLOW[1]

P. D. Butler,[2] W. A. Hamilton, L. J. Magid,[3] T. M. Slawecki,[4] J. B. Hayter, and B. Hammouda[4]

The main applications of viscoelastic surfactant solutions rely on their shear thinning, drag reducing, and lubricating properties. Clearly such phenomena must be governed by the fluid microstructural behavior under flow near a surface.

Near-surface small-angle neutron scattering (NS-SANS) measurements on the rodlike micelles of the mixed surfactant system cetyltrimethylammonium 3,5-dichlorobenzoate-bromide surfactants in D_2O indicate that under shear and within the first 30 μm from the surface, the rods not only align themselves in the direction of the flow but arrange themselves into a remarkably well-ordered hexagonal "crystal" oriented parallel to the surface.[5]

In order to study the extent to which this ordering is purely a surface phenomenon, SANS measurements of the bulk solutions have been made under shear using a Couette shearing device. Because observation of the first-order peaks requires a different crystal orientation than is required for observation of the second-order peaks, the existence of both peaks in these data shows (Fig. 1) that the shear-oriented hexagonal structure cannot persist into the bulk. Further attempts to fit the data with a 2D hexagonal powder model failed, indicating that the most likely bulk ordering is that of a 2D liquid with the rods oriented in the flow direction. Thus, the hexagonal structure seems to be completely driven by the proximity of the surface rather than the flow field.

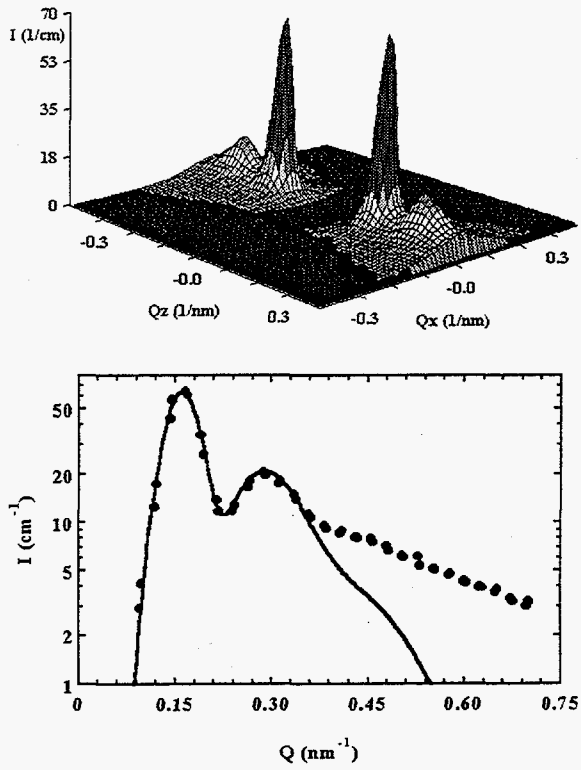

Fig. 1. Couette SANS pattern for 70:30 CTA35ClBz/CTABr in D_2O at 200 s-1. Graph shows $Q_x = 0$ slice data. Line is powder model.

1. Summary of paper: *Faraday Discussions on Complex Fluids at Interfaces, Cambridge, UK, September 18, 1996* (in press).

2. ORNL/ORISE postdoctoral research associate.

3. The University of Tennessee, Knoxville, Tenn.

4. National Institute of Standards and Technology, Gaithersburg, Md.

5. W. A. Hamilton et al., *Phys. Rev. Lett.* 72, 2219 (1994).

LIQUID-LIQUID EXTRACTIONS USING DENDRIMER-MODIFIED CO_2 TO PURIFY WATER[1]

A. I. Cooper,[2] J. D. Londono,[3] G. D. Wignall, J. B. McClain,[2] E. T. Samulski,[2] J. S. Lin, A. Dobrynin,[2] M. Rubinstein,[2] J. M. J. Frechet,[3] and J. M. DeSimone[2]

Above its critical point, carbon dioxide forms a supercritical fluid (SCF), which is widely used in the food industry because of its nontoxic nature. The use of supercritical CO_2 in the polymer industry has also provoked much interest, as it promises to be an environmentally responsible replacement for the organic solvents traditionally used in polymerizations and processing. Typically, only two classes of polymers have shown significant solubility in CO_2 under practicable conditions: amorphous fluoropolymers and polysiloxanes.

Small-angle x-ray scattering (SAXS) and small-angle neutron scattering studies have shown that partially fluorinated, amphiphilic block copolymer surfactants can aggregate into micelles in supercritical CO_2 and that CO_2-insoluble material can be solubilized in the core of these particles.[4]

Dendrimers are highly branched polymers which form a range of guest-host systems, whereby guest molecules may be trapped in a permeable dendritic core which is surrounded by a relatively dense shell. Reported here are the first synthesis and SAXS characterizations of a unimolecular dendritic micelle, which can solubilize polar ionic species in CO_2.

Figure 1 shows the SAXS data which confirm that the molecular weight (33.5 kg/mol) and radius of gyration (30 Å) are consistent with the micelle containing only one molecule. Remarkably, it was found that the dendritic micelle can transfer ionic species (e.g., methyl orange, a CO_2-insoluble dye) from aqueous solution into CO_2 without forming a water-in-CO_2 microemulsion. These experiments demonstrate that surfactant-modified CO_2 can be used dramatically to enhance the applicability of supercritical fluid extractions using environmentally benign CO_2 to replace some of the billions of pounds of organic solvents used every year in extraction and cleaning applications.

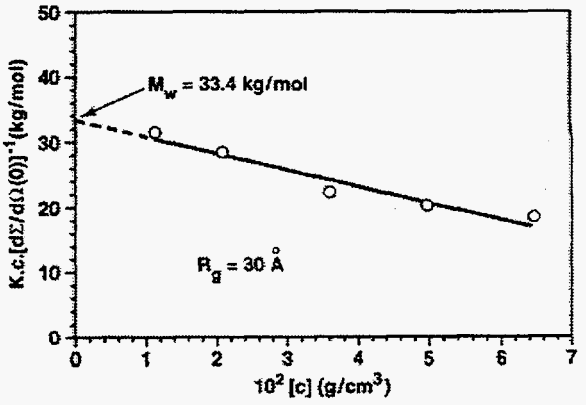

Fig. 1. SAXS characterization of a fourth-generation hydrophilic dendrimer, functionalized with perfluoroether chains to generate a CO_2-soluble unimolecular dendritic micelle.

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1. Summary of paper: *Nature* (in press).
2. University of North Carolina at Chapel Hill, Chapel Hill, N.C.
3. Cornell University, Ithaca, N.Y.
4. J. B. McClain, *Science* **274**, 2049 (1996)

PHASE BEHAVIOR AND MORPHOLOGY OF POLY(ETHYLENE OXIDE) BLENDS[1]

S. Balijepalli,[2] J. M. Schultz,[2] and J. S. Lin

Poly(ethylene oxide) (PEO) is one of the most extensively studied linear polymers. The complexity of crystallization behavior and morphology possibly comes from the existence of functional hydroxyl end groups. The growth and transformation of nonintegral folding chain crystals and integral folded chain crystals depend on the molecular weight (*MW*) of blend components, the possible network of hydrogen bonding at the surface that decreases the surface energy, and the thickening and thinning of crystals during transformation.

Time-resolved, in situ small-angle x-ray scattering (SAXS) studies have been performed on the crystallization behavior and morphology of PEO blends of high molecular weight (*MW* = 270 K, polydispersity = 1.1, equilibrium T_m = 70.2°C) and low molecular weight (*MW* = 5 K, polydispersity = 1.05, equilibrium T_m = 63.2°C). Complementary differential scanning calorimetry (DSC) with a Perkin Elmer DSC7 system and optical microscopy (OM) with a Nikon Microphot-SA microscope in conjunction with a Mettler hot stage were carried out for further confirmation of SAXS results.

At low crystallization temperatures (<40°C), both components cocrystallize into a common crystal lattice. The thickness of the cocrystal is found to vary with the blend composition. For a blend containing a high fraction of low *MW*, the cocrystals are thin, corresponding to the folding of the long chain molecules of high *MW* into the smaller. At higher compositions of high *MW* fraction, the cocrystals are thicker, resembling a crystal of the pure high MW fraction. At higher crystallization temperatures (>45°C), dynamic phase separation of the two components was observed. Time-resolved SAXS data for the blends show that the two components cocrystallize first to form a defect structure. The components in the cocrystal subsequently thin and thicken, leading to a dynamic phase splitting of the blend components. The long chain crystals are found to thicken, a process which does not occur in the neat polymer, and the short-chain crystals thin down to exclude chain ends from the crystal lattice. This phase splitting is shown to lead to phase segregation, and then both components crystallize in phase-segregated areas. The DSC and OM techniques confirm the mechanism of phase segregation.

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1. Summary of paper: *Macromol.* **29**, 6601 (1996).
2. University of Delaware, Newark, Del.

"WINDOW OF MISCIBILITY" IN THE PHASE BEHAVIOR OF BLENDS OF ISOTACTIC POLYPROPYLENE WITH RANDOM POLYOLEFIN COPOLYMERS[1]

P. A. Weimann,[2] J. D. Londono,[3] Y. Melnichenko,[4] and G. D. Wignall

Saturated hydrocarbon polymers (polyolefins) such as polypropylene represent the largest single segment of the polymer market. In commercial practice, polyolefins are often blended (alloyed) together, and such materials are used in a wide range of practical applications. However, the ability to control their properties has been handicapped by the absence of a consensus in understanding why most polyolefins are immiscible at the molecular level. Small-angle neutron scattering (SANS) is the premier technique for studying polyolefin compatibility and may be used to establish criteria to produce homogenous polyolefin mixtures. Miscibility is controlled by a balance of entropic and enthalpic factors, and because polyolefins are composed of carbon and hydrogen, they are governed solely by weak (van der Waals) interactions. Thus, the free energy of mixing (H_{mix}) is very sensitive to entropic effects, which can be characterized by the statistical segment length (a), normalized to a reference volume (≈120 Å^3), which takes into account the volume of the chain and is related to the overall size or radius of gyration ($R_g \sim a$). It has been suggested[5] that mismatches in the segment length between polymers should result in phase separation, while matching the segment lengths between the components should maximize miscibility.

In order to test this hypothesis, a series of blends of isotactic polypropylene (i-PP) with model copolymers of ethyl-ethylene$_{XX}$ and ethylene$_{(1\text{-}XX)}$ [where XX is the % of polyethylethylene (PEE)] were prepared. When the PEE content is between 73% (a = 6.4 Å) and 90% (a = 5.2 Å), the segment lengths of the copolymer are close to that of i-PP (a = 5.6 Å), and the SANS data in the melt (T = 180°C) can be fitted via the de Gennes random phase approximation. The fitted values of the interaction parameter ($\chi \sim 10^{-4}$) indicate miscibility.[1] When the PEE content is lower, the segment lengths are no longer "matched," and the blends are either marginally (XX = 62%) or strongly (XX = 46%) phase segregated. To our knowledge, this is the first time that a window of miscibility in which random copolymers form single-phase mixtures with polypropylene has been established, and this is a first step to establishing the criteria for producing miscible polyolefin blends.

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1. Summary of paper: *Macromolecules* (in press).
2. University of Minnesota, Minneapolis, Minn.
3. Chemical and Analytical Sciences Division, ORNL.
4. ORNL/ORISE postdoctoral research associate.
5. F. S. Bates and G. H. Frederickson, *Macromol.* 27, 1065 (1994).

KINETICS OF POISEUILLE SHEAR-INDUCED SURFACE ORDERING IN A SOLUTION OF THREADLIKE MICELLES

W. A. Hamilton, P. D. Butler,[1] L. J. Magid,[2] Z. Han,[2] J. B. Hayter, and T. M. Slawecki[3]

The rheological properties of complex colloidal fluids depend largely on microscopic structures established under flow. Using near-surface small-angle neutron scattering (NS-SANS), it has been observed that under such Poiseuille shear conditions, remarkable near-surface hexagonal ordering occurs in the charged highly extended threadlike micelles formed in dilute aqueous solutions of the mixed surfactant system cetyltrimethylammonium 3,5-dichloro-benzoate/ bromide.[4] This micellar arrangement is strongly oriented with respect to the surface and dramatically minimizes their interference under flow as they move past the surface and each other in the boundary layer.

Obviously, the kinetics of a near-surface state of this type would be a critical factor in surface-dominated flow characteristics such as drag and lubrication. Measurements on the ORNL 30-m SANS only allowed an ~15-min upper limit on the decay time. By coordinating computer control of the Poiseuille shear sample cell and the recently developed "time-slicing" capability of the NIST[3] NG3 SANS in a cycling mode, the first measurements of the decay time kinetics for a near-surface state after the cessation of flow have been made. The results for two peaks in the structure's neutron diffraction pattern, the **01** (normal to the surface) and the weaker **10** (at 60° to the surface) are shown in Fig. 1.

The time constant of decay is 3.5 seconds. This is *two order of magnitude* faster than that observed for bulk shear alignments.[5] Further, although the relative strength of the **01** peak and its persistence

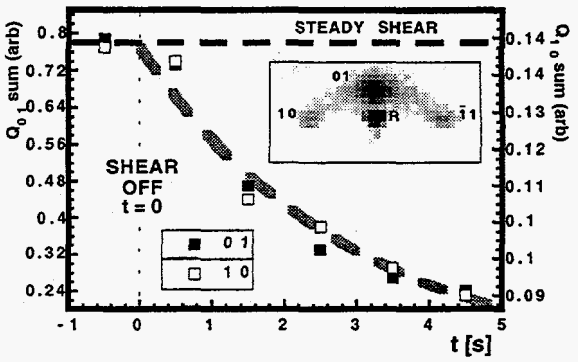

Fig. 1. Decay of integrated 01 and 10 diffraction peak intensities (shown in inset) after cessation of flow ($t = 0$).

to higher flow rates (and a presumably more turbulent regime) in steady state measurements[4] have seemed to indicate that the hexagonal structure is better ordered and in some sense "stiffer," and in the shear gradient (surface normal) direction, both peaks decay at the same rate. This disappearance of any apparent difference with the cessation of flow suggests some "micro-rheological" hydrodynamic effect acting within a few tens of micron of the surface.

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1. ORNL/ORISE postdoctoral research associate.
2. The University of Tennessee, Knoxville, Tenn.
3. National Institute of Standards and Technology, Gaithersburg, MD.

4. W. A. Hamilton et al., *Phys. Rev. Lett.* **72**, 2219 (1994)
5. P. D. Butler et al., *J. Phys. Chem.* **100**, 442 (1996).

OPTIMIZATION OF A BONSE-HART ULTRASMALL ANGLE NEUTRON SCATTERING FACILITY BY ELIMINATING THE ROCKING CURVE WINGS[1]

M. Agamalian,[2] R. Triolo,[3] and G. D. Wignall

The ORNL ultrasmall angle neutron scattering (USANS) facility at the High-Flux Isotope Reactor (HFIR) has been upgraded recently using the Bonse-Hart technique. A Si(111) triple-bounce channel-cut monochromator and analyzer have been installed instead of previously used single-bounce crystals. The full width at half-maximum of the rocking curve is about 1.5 arc s, and the wavelength of the primary neutron beam is 2.59 Å. It has been demonstrated that due to the low neutron absorption of Si, the wings of the rocking curve are generally contaminated by neutrons propagating inside and diffracting from the back face of the long wall of the channel-cut crystal. This parasitic intensity has been eliminated by cutting a groove in the long wall and inserting a cadmium absorber (0.6-mm thick). This modification effectively suppresses the wings of the rocking curve by a factor of ~100, and deep-surface etching produces further reduction; thus, an overall gain in the signal-to-noise ratio of the instrument is about three orders of magnitude (Fig. 1). The upgraded facility has been tested using several samples, including a polystyrene latex with a radius of 2.5×10^4 Å, as determined by optical microscopy. The average radius calculated from USANS data is 2.48×10^4 Å, in good agreement with the independently determined dimensions. The minimum accessible scattering vector of the upgraded USANS facility

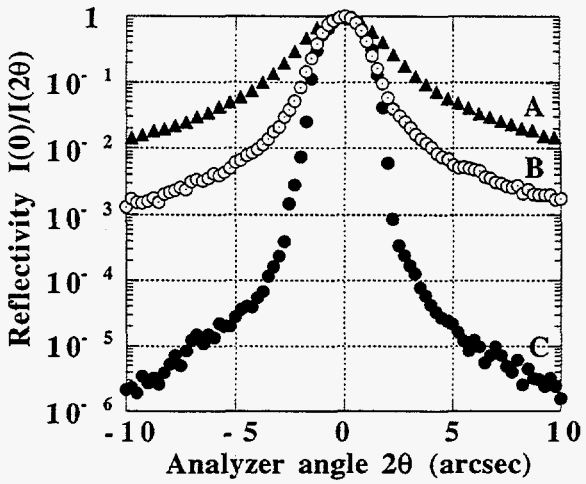

Fig. 1. Rocking curves: (a) single-/single-bounce scheme; (b) triple-/triple-bounce scheme; and (c) triple-/triple-bounce scheme with surface-etched channel-cut crystals containing Cd absorber.

is $Q_{min} = 2 \times 10^{-5}$ Å^{-1} which corresponds to a maximum resolvable real-space dimension of $2\pi/Q \sim 3 \times 10^5$ Å (30 μm).

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1. Summary of paper: *J. Appl. Cryst.* **31**, 1, (1997).
2. ORNL/ORISE postdoctoral research associate.
3. Guest scientist from the University of Palermo, Palermo, Italy.

DIMENSIONS OF POLYMER CHAINS IN POOR SOLVENTS[1]

Y. B. Melnichenko[2] and G. D. Wignall

The dimensions of macromolecules in organic solvents depend crucially on the sign and magnitude of the interactions between the chain segments and the molecules of the surrounding liquid. At a particular temperature (Θ), the solvent-solute and solute-solute interactions, which have opposite signs, are precisely balanced; therefore, the radius of gyration (R_g) corresponds to the dimensions of volumeless noninteracting polymer coils. In the poor solvent regime ($T << \Theta$), the attractive and repulsive forces are no longer balanced, and R_g is believed to collapse.

Most theoretical calculations of R_g at the critical demixing temperature $T_c < \Theta$ have been based on de Gennes' concept that at the critical point, polymer chains do not interpenetrate significantly,[3] leading to a prediction that the chains are collapsed at T_c [i.e., $R_g(T_c) << R_g(\Theta)$]. Providing definitive experimental data on the size of polymer chains in relatively concentrated solutions at the critical point has remained a challenge for the past decade because of the difficulties of separating the inter- and intrachain contributions to the structure. However, it has been demonstrated[1] recently that the R_g of the polymer chains in concentrated solutions can be obtained via small-angle neutron scattering (SANS) techniques. The results are illustrated in Fig. 1 which shows the temperature dependence of R_g for polystyrene chains in deuterium-labeled cyclohexane (to provide SANS contrast). It may be seen that the predicted[3] decrease in R_g is not observed as $T \rightarrow T_c$, and this indicates that critical polymer solutions can no longer be considered as an ensemble of collapsed, noninterpenetrating chains. Instead, the diverging thermodynamic fluctuations near T_c lead to the formation of distinct microdomains, representing strongly interpenetrating molecules. Further research shows that polystyrene-acetone solutions behave similarly; therefore, this is a general result which is not restricted to cyclohexane solutions. This observation is of fundamental importance for understanding not only the physical properties of polymer solutions but also the phase transitions of proteins in biological systems.

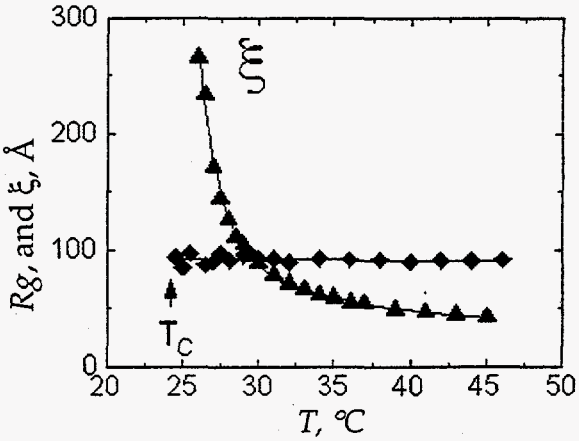

Fig. 1. R_g and correlation length (ξ) for polystyrene in d-cyclohexane vs. temperature.

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1. Summary of paper: *Phys. Rev. Lett.* **78**, 686 (1997).
2. ORNL/ORISE postdoctoral research associate.
3. P.-G. de Gennes, p. 115 in *Scaling Concepts in Polymer Physics*, Cornell University Press, Ithaca, N.Y., 1979.

DEMONSTRATION OF MICELLE FORMATION AT A CRITICAL DENSITY FOR BLOCK-COPOLYMER SURFACTANTS IN CARBON DIOXIDE[1]

G. D. Wignall, J. D. Londono,[2] R. Triolo,[3] J. B. McClain,[4] D. E. Betts,[4] and J. M. DeSimone[4]

Above its critical point, carbon dioxide forms a supercritical fluid (SCF), which promises to be an environmentally responsible replacement for the organic solvents traditionally used in polymerizations. However, many polymers are insoluble in CO_2, and this necessitates the use of block copolymer emulsifying agents (surfactants) to solubilize the CO_2-phobic material. These consist of two different polymers covalently bonded together. The different ends are either attracted to, or repelled by, CO_2 and thus form micelles which suspend the growing polymer chains inside and shield them from contact with the supercritical solvent. These aggregates comprise typically a dense core formed by the insoluble blocks, surrounded by a shell of solvated blocks. The micelles have been shown to be capable of solubilizing CO_2-phobic materials[1] thus promoting polymerization processes.

As the density of CO_2 is increased, the solvation of the two components of a diblock copolymer becomes greater, which should result in a decrease in aggregation and eventually unimers (i.e., single molecules). Thus, the existence of a critical micelle density (CMD) is anticipated,[1] and recent experiments demonstrate this new phenomenon for the first time. Fig. 1 shows the pressure dependence of the small-angle neutron scattering (SANS) data from a polyvinyl acetate-b-polyfluro-octyacrylate (PVA-b-PFOA) diblock copolymer at constant concentration (6% wt/v). The cross section increases by over an order of magnitude as the pressure decreases from 4000 to 2400 psi, signaling the transition from unimers to micellar aggregates. A unique attribute of SCFs is that the solvent strength is easily tunable with changes in the system density, and the CMD constitutes a new concept in colloid and surface chemistry.

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1. Summary of paper: *Science* **274**, 2049, (1996).
2. Chemical and Analytical Sciences Division, ORNL.
3. Guest scientist from Palermo University, Palermo, Italy.
4. University of North Carolina at Chapel Hill, Chapel Hill, N.C.

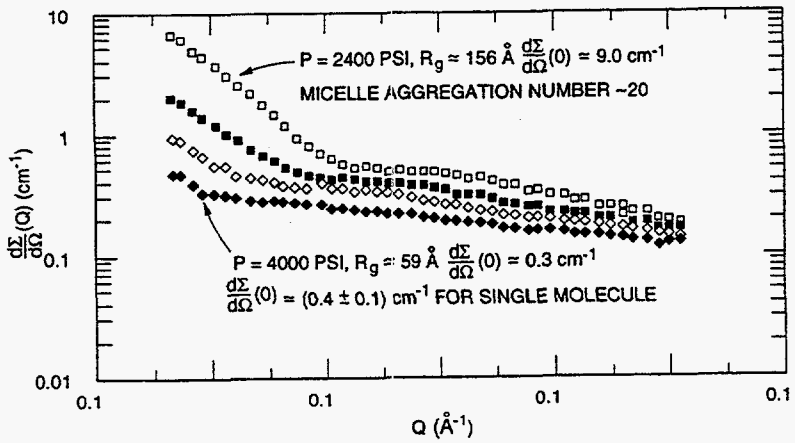

Fig. 1. $d\Sigma/\Omega(Q)$ for 6% (w/v) PVA-b-PFOA block copolymers in CO_2. At high pressures, the scattering arises from single molecules; as the pressure is lowered, micelles form below a critical density.

SMALL-ANGLE NEUTRON SCATTERING STUDY OF OF THE FLUX-LINE LATTICE IN YNi_2B_2C

M. Yethiraj

Rare-earth nickel borocarbides of the type RNi_2B_2C (R = rare-earth) were discovered[1] to be superconducting in 1994. Shortly thereafter, it was found that some of these compounds containing a magnetic rare-earth ion exhibited coexistence[2] of magnetic order with superconductivity. It is seen that the rare-earth ions order in the magnetic state; Ni ions do not appear to have a moment. The interplay between magnetism in the rare-earth nickel borocarbides and superconductivity is a topic of considerable interest, because magnetism and superconductivity are typically expected to be competing interactions. It is essential, however, to know the properties of the nonmagnetic compound so that the properties that are exclusive to magnetic compounds can be deduced. In order to do this, the compound YNi_2B_2C, which does not order magnetically, has been studied. This is the first flux-line lattice study on the nonmagnetic rare-earth nickel borocarbide using small-angle neutron scattering (SANS). Neutrons, having a magnetic moment, interact with the field modulations caused by an array of flux lines. Bragg scattering of the neutrons from this ordered array of vortices makes it possible to study the bulk structure of the lattice. Further, the intensity of the Bragg scattering is inversely proportional to the fourth power of the London penetration depth in the material making it possible to determine this quantity very accurately. A square lattice is observed with the applied field parallel to the c-axis of the YNi_2B_2C crystal and is quite remarkable in its stability over a very wide range of temperature and field. An increase in the disorder of the vortices is observed as the field is increased resulting in a large reduction in the Bragg intensity at higher fields. It is possible that this precedes a change in symmetry of the flux lattice from square to hexagonal.

These results[3] are contrary to the conclusions of the vortex lattice study[4] in magnetic $ErNi_2B_2C$, where the researchers decided that the square symmetry of the flux lattice was related to the magnetic structure in the compound.

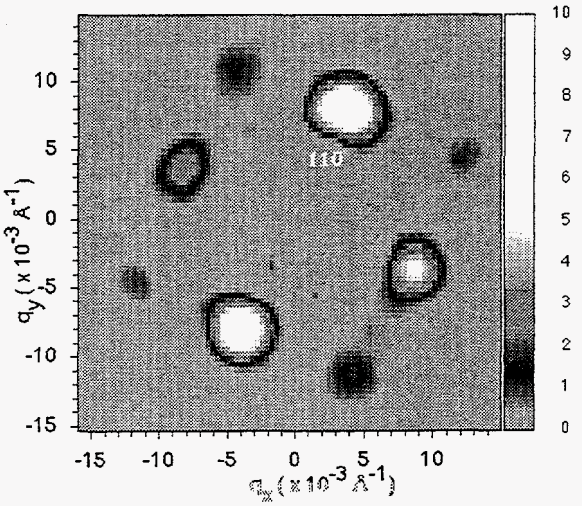

Fig. 1. The observed flux lattice in a single crystal of YNi_2B_2C with the applied field parallel to the c-axis of the crystal.

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1. C. Mazumdar et al., *Solid State Commun.* 87, 413 (1994); R. Nagarajan et al., *Phys. Rev. Lett.* 72, 274 (1994); R. J. Cava et al., *Nature* **367**, 146 (1994).

2. C. V. Tomy et al., *Physica B* **213 & 214**, 139 (1995); A. I. Goldman et al., *Phys. Rev. B* **51**, 678 (1995).

3. M. Yethiraj et al., *Phys. Rev. Lett.* **78**, 4849 (1997).

4. U. Yaron et al., *Nature* **382**, 236 (1996).

NEUTRON SCATTERING FROM A TANK SLUDGE MODEL SYSTEM

P. D. Butler,[1] M. L. Balmer, [2] P. A. Smith,[2] M. Agamalian,[1] and W. A. Hamilton

The unforgiving rheology of inorganic colloidal sludges represents a daunting problem in the processing of 60 million gallons of radioactive tank wastes stored at the DOE's Hanford site. During processing, these sludges will experience various conditions of shear and pressure filtration (or sedimentation) which can alter their flow properties in unwelcome ways—clogging pipes and making their transport difficult or impossible.

In order to understand better the behavior of these sludges under process conditions, an ORNL/PNNL collaboration has designed and constructed a new pressure filtration cell for small-angle neutron scattering (SANS) and ultrasmall angle neutron scattering (USANS), allowing the first direct measurements of how the microstructures in concentrated clay suspensions respond to such processing.

In this initial study, slurries of boehmite (AlOOH, a main ingredient in tank waste) have been examined. Measurements on ORNL's upgraded USANS facility[3] have revealed correlation lengths prior to filtration on the order of 3-4 μm, with the higher concentrations (15% vs. 6% vol) having smaller correlation lengths as predicted by theory. After 12 hours of pressure filtration at 40 psi, the USANS intensity falls dramatically indicating a collapse of the network structure of the boehmite platelets in the slurry. Normal SANS measurements of the cake (the region adjacent to the filter) formed from a 3% solution of pH 4 with 1-M electrolyte content indicate a small, but significant anisotropy which does not exist in the regions further away from the filter. This indicates that even at these high electrolyte concentrations when electrostatic shielding allows closer contact, the platelets can still slide over each other sufficiently to orient themselves. Besides the anisotropy, the scattering curves from measurements in the cake region, adjacent the filter, are distinctly different from those from regions away from the filter. This is probably due to the network structure being completely eliminated in the cake, while the regions further from the filter still support a compressed network.

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1. ORNL/ORISE postdoctoral research associate.

2. Pacific Northwest National Laboratory, Richland, Wash.

3. M. Agamalian et al., "Optimization of a Bonse-Hart Ultrasmall Angle Neutron Scattering Facility by Eliminating the Rocking Curve Wings," this report.

NEW COLD NEUTRON SCATTERING CAPABILITIES AT HFIR

G. D. Wignall

A high-performance cold source and several new state-of-the-art neutron scattering facilities will be installed at HB-4. Four instruments, including a cold neutron triple-axis spectrometer (CNTAS), a biological station, a neutron reflectometer, and a 35-m high-resolution (up to 10 Å) small-angle neutron scattering (SANS) spectrometer (SANS-1), are currently being designed. The projected flux at the SANS-1 sample position is comparable to the best existing SANS facility in the world, currently D11/D22 at the Institut Laue-Langevin (ILL) as shown in Fig. 1. This flux is an order of magnitude higher than available at current U.S. SANS facilities. A second SANS instrument (SANS-2) is planned in the future, which will achieve even higher intensities for medium-resolution studies of smaller structures (up to 100 Å).

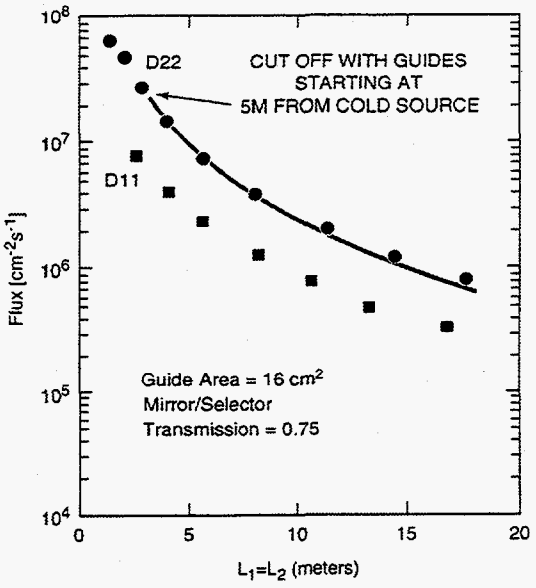

Fig. 1. ORNL flux simulation (4/97) with Monte Carlo neutron photon cold neutron library H2-cross sections (λ = 10 Å, $\Delta\lambda/\lambda$ = 10%).

A CNTAS is a superior instrument for high-resolution and small momentum transfer measurements, and the new spectrometer will be comparable to the best in the world. It will function both in a conventional or polarized scattering mode. This instrument will have a dramatic impact on broad areas of condensed matter physics, including disordered systems, magnetism, and superconductivity.

In the last decade, neutron reflectrometery has emerged as a powerful probe of surface and interface structures, including thin-film superconductors, soap films, polymer interfaces, and model biological lipid membranes. Location of the existing reflectometer at HFIR in the cold neutron hall will double the instrument's resolution and significantly reduce background, while increasing the effective incident neutron intensity by an order of magnitude. These improvements will make this instrument the most capable of its kind in the world.

The planned facilities will enhance the competitiveness of U.S. researchers in a wide variety of disciplines, including condensed matter physics, materials science, chemistry, and biology. A broad spectrum of sample environments, including low- and high-temperature and high-pressure capabilities, novel shear and extensional flow fields, and applied electric and magnetic fields, will be employed. The proposed instruments will provide unsurpassed facilities for cold neutron research, and a significant increase in the number of users is expected.

Chapter 3

Synthesis, Processing, and Characterization of Materials

Superconductivity

EPITAXIAL $YBa_2Cu_3O_7$ ON BIAXIALLY TEXTURED (001) Ni: AN APPROACH TO HIGH CRITICAL CURRENT DENSITY SUPERCONDUCTING TAPES[1]

D. P. Norton, A. Goyal,[2] J. D. Budai, D. K. Christen, D. M. Kroeger,[2] E. D. Specht,[2] Q. He,[3] B. Saffian,[3] M. Paranthaman,[4] C. E. Klabunde,[5] D. F. Lee,[2] B. C. Sales, and F. A. List[2]

Since the discovery of high-temperature superconductivity (HTSc) in cuprate materials, significant efforts have focused on developing a high-current superconducting wire technology for applications at 77 K.[6] Although randomly oriented polycrystalline HTSc materials have low critical current densities, J_c, $YBa_2Cu_3O_7$ (YBCO) thin films grown epitaxially on single-crystal oxide substrates exhibit J_c values > 1 MA/cm² at 77 K.[7] In order to achieve a wire or tape with a high J_c, the crystallographic orientation of the HTS superconducting wire or tape must possess a high degree of both in-plane and out-of-plane grain alignment over the conductor's entire length.

An approach for achieving in-plane aligned, high critical current YBCO films on long-length substrates has been developed. A biaxially textured (001) Ni tape, formed by recrystallization of cold-rolled pure Ni, is used as the initial, in-plane aligned substrate. A (001)-oriented oxide buffer layer architecture is then epitaxially grown that maintains the sharp crystallographic cube texture of the metal substrate while providing a barrier to chemical interaction with the Ni. Subsequent growth of YBCO on this structure, referred to as a rolling-assisted, biaxially textured substrate (RABiTS), results in c-axis oriented, in-plane aligned films with J_c's as high as 700,000 A/cm² at 77 K, as indicated in Fig. 1. This result represents a viable approach for producing long-length superconducting tapes for high-current, high-field applications at 77 K.

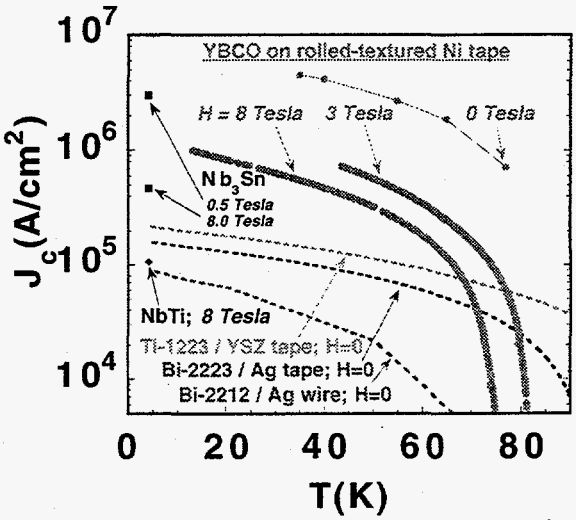

Fig. 1. The critical current density for YBCO-based RABiTS structure as a function of temperature.

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1. Summary of paper: *Science* **274**, 755 (1996).
2. Metals and Ceramics Division, ORNL.
3. The University of Tennessee, Knoxville, Tenn.
4. Chemical and Analytical Sciences, ORNL.
5. ORNL retiree.
6. Thomas P. Sheahen, p. 317 in *Introduction to High-Temperature Superconductivity*, Plenum Press, N.Y., 1994.
7. D. H. Lowndes et al., *Phys. Rev. Lett.* **74**, 2355 (1995).

DEPOSITION OF BIAXIALLY ORIENTED METAL AND OXIDE BUFFER-LAYER FILMS ON TEXTURED Ni TAPES: NEW SUBSTRATES FOR HIGH-CURRENT, HIGH-TEMPERATURE SUPERCONDUCTORS[1]

Q. He,[2] D. K. Christen, J. D. Budai, E. D. Specht,[3] D. F. Lee,[3] A. Goyal,[3] D. P. Norton, M. Paranthaman,[4] F. A. List,[3] and D. M. Kroeger[3]

A multidisciplinary research effort at ORNL recently demonstrated a new, enabling approach for the production of high-current, high-temperature superconducting (HTSc) wires.[5] An essential component of this approach is the epitaxial deposition of oxide buffer layers and superconductor coatings on a sharply biaxially textured metallic nickel tape. The buffer layers act as both a template for epitaxy and a chemically compatible interface between the reactive metal and the desired HTSc coating.

In the present work, methods have been developed for the epitaxial deposition of various buffer layers using rf or dc magnetron sputtering—a vapor deposition technique that is widely used and familiar to industry. In particular, CeO_2 is a desirable buffer layer for $YBa_2Cu_3O_7$ because of its good lattice match and chemical compatibility at typical HTSc deposition temperatures of 750–800°C. Here, epitaxial layers of CeO_2 on nickel have been successfully deposited using two different techniques. In both processes, the principal achievement is the prevention of NiO formation during buffer-layer deposition, because its presence destroys epitaxial alignment.

In the first approach, a thin epitaxial layer of Pd was deposited on Ni at temperatures as low as 25°C, followed by growth of CeO_2 at somewhat elevated temperatures and in an oxidizing atmosphere of a 6-mTorr $Ar/10\%O_2$ gas mixture. The results show that optimal CeO_2 alignment, which is comparable to the underlying Ni texture, occurs near 300°C. This optimum temperature is apparently related to competing effects of thermally enhanced CeO_2 order and interdiffusion of Pd and Ni.

In the second approach, an initial 10–30-nm layer of CeO_2 was sputtered directly onto the bare Ni surface in the presence of a reducing $Ar/4\%H_2$ gas ambient, followed by additional deposition in $Ar/10\%O_2$. This procedure produced excellent epitaxy and should be generally useful provided the relative stabilities of the reactive metal surface and the oxide coating are sufficiently different.

These results provide a basis for the production of a new class of inexpensive, large-scale biaxially textured substrates for HTSc wires, as well as for novel applications in a variety of thin-film technology areas.

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1. Summary of paper: *Physica C* **275**, 155 (1997).
2. Graduate student from The University of Tennessee, Knoxville, Tenn.
3. Metals and Ceramics Division, ORNL.
4. Chemical and Analytical Sciences Division, ORNL.
5. D. P. Norton et al., *Science* **274**, 755(1996).

SUPERCONDUCTING TRANSPORT PROPERTIES OF HIGH-J_c BIAXIALLY ALIGNED $YBa_2Cu_3O_{7-\delta}$ DEPOSITS ON METALLIC TAPE SUBSTRATES[1]

D. K. Christen, H. R. Kerchner, D. P. Norton, A. Goyal,[2] J. D. Budai, R. Feenstra, Q. He,[3] C. E. Klabunde, D. M. Kroeger,[2] D. F. Lee,[2] F. A. List,[2] M. Paranthaman,[4] B. Saffian,[5] E. D. Specht,[2] and M. F. Chisholm

Applications of high-temperature superconductors (HTSc) for power devices will require the conduction of large currents in substantial magnetic fields, preferably operating at liquid nitrogen temperatures (e.g., in the range 64–77 K). Recently, a new approach for the production of high critical current density J_c wires, based on the deposition of biaxially aligned $YBa_2Cu_3O_7$ coatings on thermomechanically textured nickel tapes, was demonstrated.[6,7] The superconducting electrical transport has been measured on a series of short samples, with attention both to fundamental characteristics and to properties relevant to a tape-conductor technology.

Comparative studies were made with epitaxial thin films on single-crystal oxide substrates, well known to be "benchmark" high-J_c materials. Results show that $YBa_2Cu_3O_7$ films on textured metal substrates exhibit high-field properties that match or exceed those of the best control samples. The flux-pinning defects necessary for these properties appear to result from intrinsic HTSc–substrate interactions during film growth. An important issue for wire applications is the ability to carry large absolute currents, which requires the retention of properties in thick HTSc deposits. Figure 1 shows the measured thickness dependence, compared with a practical operation criterion. These findings demonstrate feasibility for the production of a new class of enabling HTSc conductors, capable of operating in liquid nitrogen and in the presence of magnetic fields—as required for applications in motors, generators, and magnetic energy-storage devices.

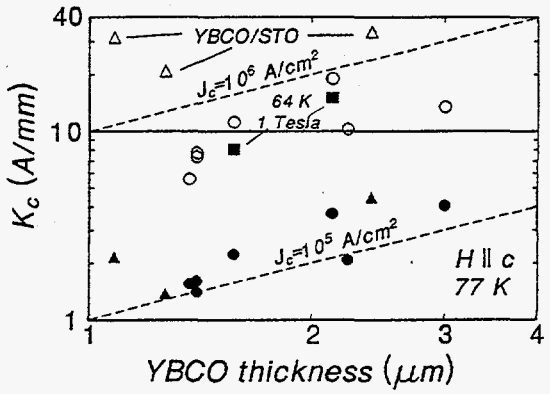

Fig. 1. The loss-free current K_c carried per unit width of tape for different YBCO layer thicknesses at 77 K. Open symbols: zero applied field. Closed symbols: 1-T applied field. Solid line: K_c = 10 A/mm, a proposed practical operation criterion. Squares: data in 64-K liquid nitrogen.

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1. Summary of paper: *Czechoslovak J. Phys.* **46**, 1531 (1996).
2. Metals and Ceramics Division, ORNL.
3. Graduate student from The University of Tennessee, Knoxville, Tenn.
4. Chemical and Analytical Sciences Division, ORNL.
5. The University of Tennessee, Knoxville, Tenn.
6. D. P. Norton et al., *Science* **274**, 755 (1996).
7. A. Goyal et al., *Appl. Phys. Lett.* **69**, 1795 (1996).

ALTERNATING CURRENT LOSSES IN BIAXIALLY TEXTURED $YBa_2Cu_3O_{7-\delta}$ FILMS DEPOSITED ON Ni TAPES[1]

H. R. Kerchner, D. P. Norton, A. Goyal,[2] J. D. Budai, D. K. Christen, D. M. Kroeger,[2] Q. He,[3] M. Paranthaman,[4] D. F. Lee,[2] B. C. Sales, F. A. List,[2] and R. Feenstra

Although there is a high level of interest in high-T_c superconducting cable for future applications, presently available materials are limited because magnetic fields reduce their current-carrying capacities. Single-crystalline and grain-aligned $YBa_2Cu_3O_{7-\delta}$ (YBCO) have long appeared to be attractive solutions because of their field strength, and YBCO films grown on rolling-assisted biaxially textured substrates (RABiTS) can carry very high current densities.[5]

Although dc electrical currents less than the critical value flow through superconductive material with minimal loss, ac current gives rise to loss, even without exceeding the critical current. The current density distributes itself so that the induced magnetic field is excluded from the central region of the superconductive material, but not from the edge regions where the peak current densities are limited to the critical magnitude, J_c. A theoretical assessment of hysteretic ac loss during current transport was developed by W. T. Norris.[6]

The ferromagnetic Ni in the textured substrate very near the current-carrying material provides another potential source of ac loss. Observations indicate that the Ni substrate magnetizes parallel to the tape direction. The field, due to the transport current, rotates magnetization rather than enlarges and reduces domain volumes. The confinement of the field within the Ni protects the YBCO film and permits the loss-free flow of a high-current density.

Although the loss data presented in Fig. 1 lie higher than the theoretical expectation (shown as a solid line), the difference is smaller than that due to a reasonable ferromagnetic contribution. The extra loss is expected to be due to thermally assisted vortex motion.

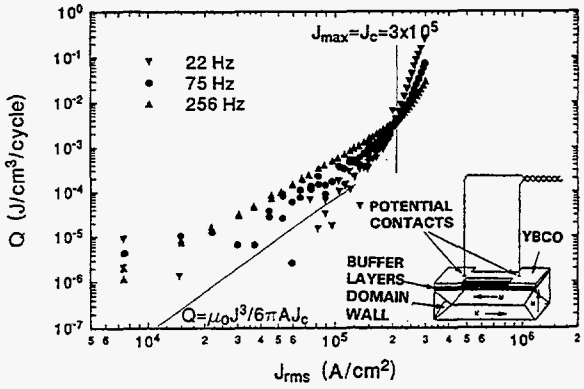

Fig. 1. Electrical power loss Q with ac current densities J through $YBa_2Cu_3O_{7-\delta}$ films on RABiTS. The inset shows a four-terminal sample diagram.

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1. Summary of paper to be published.
2. Metals and Ceramics Division, ORNL.
3. Graduate student from The University of Tennessee, Knoxville, Tenn.
4. Chemical and Analytical Sciences Division, ORNL.
5. D. P. Norton et al., *Science* **274**, 755-757 (1996).
6. W. T. Norris, *J. Phys. D, Appl. Phys.* **3**, 489 (1970).

SUPERFAST VORTEX CREEP IN $YBa_2Cu_3O_{7-\delta}$ CRYSTALS WITH COLUMNAR DEFECTS: EVIDENCE FOR VARIABLE-RANGE VORTEX HOPPING[1]

J. R. Thompson,[2] L. Krusin-Elbaum,[3] L. Civale,[4] G. Blatter,[5] and C. Feild[3]

A major impediment to applications of high-T_c superconductors is the ease of energy-consuming vortex motion. Generally columnar defects (long tracks of amorphized material) provide the most effective pinning of vortices in high-T_c materials. Their effectiveness arises from the similar linear geometry and transverse length scales, leading to quite high current densities J. Nonetheless, significant vortex motion ("giant" flux creep) still occurs, displaying a rich and varied complexity; e.g., vortices underfill the defect array at low magnetic fields and overfill it in high fields. In particular, for the underfilled case, entropic smearing of the pinning potential allows depinning of a single vortex at a comparatively low temperature, ~40 K. This also defines, in part, the "accommodation-field" boundary $B^*(T)$, which separates a regime of strong, individual pinning of vortices from a regime where vortex-vortex interactions prevail.

Near, but below, $B^*(T)$ where entropic effects weaken pinning, a vortex may find it energetically favorable to "hop" to a more-distant, vacant columnar track. This leads to particularly rapid flux motion and supercurrent decay in the HTSc. Theoretically,[6] the vortex motion maps to variable-range vortex hopping (VRH), in analogy with charge carriers in semiconductors. Figure 1 shows that the current J decays rapidly with time near 40 K. This occurs only for the underfilled case (flux density $B < B_\Phi$, the equivalent defect density) where VRH is possible. In the overfilled case ($B > B_\Phi$), the large peak in decay rate S has vanished. Other features of the vortex dynamics give further evidence for the VRH of vortices.

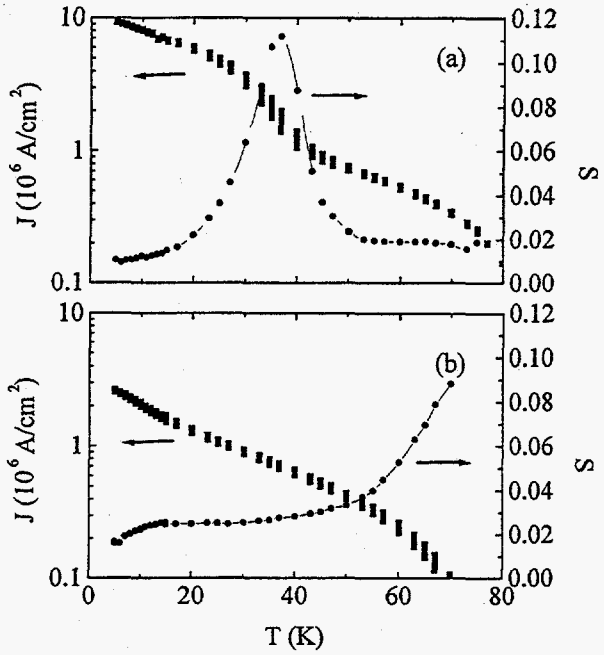

Fig. 1. Current density J and its normalized decay rate $S = d\ln(J)/d\ln(t)$, plotted vs. temperature T_c for a crystal with B_Φ = 2.4 T. (a) H = 0.5 T and (b) H = 4 T.

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1. Summary of paper: *Phys. Rev. Lett.* **78**, 3181 (1997).
2. Adjunct research and development participant from The University of Tennessee, Knoxville, Tenn.
3. IBM Watson Research Center, Yorktown Heights, N.Y.
4. Centro Atomico Bariloche, Bariloche, Argentina.
5. ETH-Hoenggerberg, Zurich, Switzerland.
6. D. R. Nelson and V. M. Vinokur, *Phys. Rev. B* **48**, 13060 (1993).

ENHANCEMENTS OF HIGHEST T_c SUPERCONDUCTORS WITH GeV PROTONS[1]

J. R. Thompson,[2] L. Krusin-Elbaum,[3] D. K. Christen, K. J. Song,[4] M. Paranthaman,[5] and J. L. Ullmann[6]

Applications of high-T_c superconductors (HTSc) will require that they conduct low-loss currents at high densities, often in a high magnetic field. Thus, magnetic flux whose motion generates heat in a superconductor must be immobilized. This is best achieved by introducing defects of optimal morphology, such as columnar defects. These amorphous latent tracks were initially formed by heavy-ion irradiation, but this method suffers from the heavy-ion limited range, which often is too small to penetrate composite conductors. To circumvent this problem, a new procedure was devised to create columnar tracks using very penetrating particles—0.8-GeV protons with a range of ~0.6 m in a HTSc. Briefly, an incident proton causes a heavy constituent nucleus, such as Bi, Hg, Tl, Pb, ..., to fission. The two fission fragments have enough energy to create a columnar track that is randomly oriented deep within the bulk material.

Broad applicability of this methodology has been demonstrated by applying it to Tl-, Hg-, and TlPb-cuprates with high T_c's > 100 K. These HTSc are also less anisotropic than Bi-cuprates and have a greater potential for high-T, high-H applications. Bulk materials and thin films, irradiated with or without "amplifier foil" overlayers, have been investigated. The columnar defects lead to significant enhancements in the current-density J. Figure 1 shows order-of-magnitude enhancements J of a thin epitaxial film of Hg-1223, measured with the magnetic field $H \parallel$ c-axis. Corresponding improvements in current transport, with J extending over a broader H-T region, were also produced in the other HTSc materials.

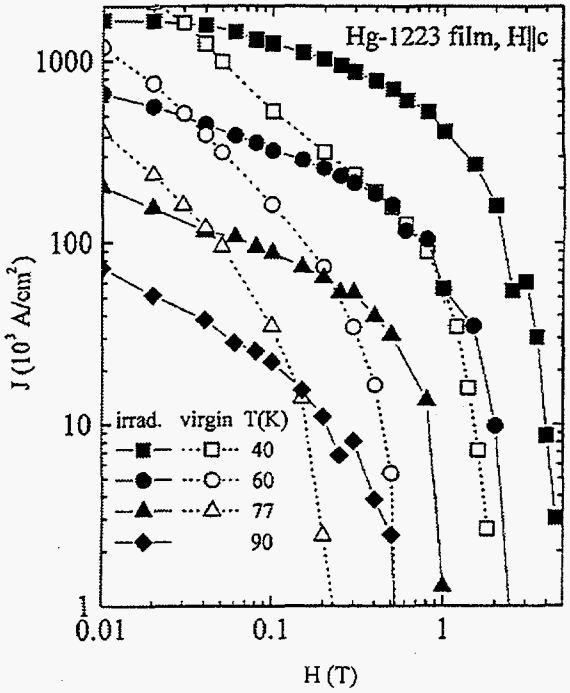

Fig. 1. The persistent current density J vs. magnetic field H, for a Hg-1223 film at the temperatures shown. The film, with a 40-μm Pb overlayer, was irradiated with 5.8×10^{16} p/cm². J is significantly increased, especially at higher fields.

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1. Summary of paper: *Applied Physics Letters* (in press).
2. Adjunct research and development participant from The University of Tennessee, Knoxville, Tenn.
3. IBM Watson Research Center, Yorktown Heights, N.Y.
4. Graduate student from The University of Tennessee, Knoxville, Tenn.
5. Chemical and Analytical Sciences Division, ORNL.
6. Los Alamos National Laboratory, Los Alamos, N. Mex.

DOPING OF THE COPPER-OXYGEN PLANES IN HIGH-T_c SUPERCONDUCTORS: DIRECT OBSERVATION OF DOPING-INDUCED IN-GAP STATES[1]

R. Feenstra, T. Matsumoto,[2] and T. Kawai[2]

In the high-temperature superconductor (HTSc) cuprates, CuO_2 planes comprise the electronically active part of the multilayered structure. Doping effects induced by bond-chemical charge transfer modulate the electron density and distribution on the CuO_2 planes, giving rise to a local response which is, at once, structure dependent and general—assuming the doping can be quantified as an extrinsic parameter and the planes themselves remain stoichiometric. It is believed that these effects are closely related to the origin of HTSc. Doping-induced variations have been studied in the local electronic structure of CuO_2 planes in a simple HTSc copper-oxide, probed directly by scanning tunneling microscopy-spectroscopy (STM-STS). The experiments were performed by probing epitaxial surfaces of the infinite-layer compound $Sr_{1-x}A_xCuO_2$ after in situ deposition, variably doped via substitutions A (Ca, La) on the Sr site. Making use of the fact that STM-STS locally probes states near the Fermi energy E_F (given by the sign and magnitude of the bias potential V), systematic variations in the insulating gap width were observed as a result of the substitutions—indicating doping-induced in-gap states (Fig. 1). The variations are consistent with a bond-valence-sum analysis of the lightly doped regime through basic dopant → in-gap state correlations, featuring solutes (La) as well as defects (Sr vacancies). It is inferred that doped electrons and holes lead to distinct modifications of the parent electronic structure, suggesting distinct effects on the effective electron-electron interaction.

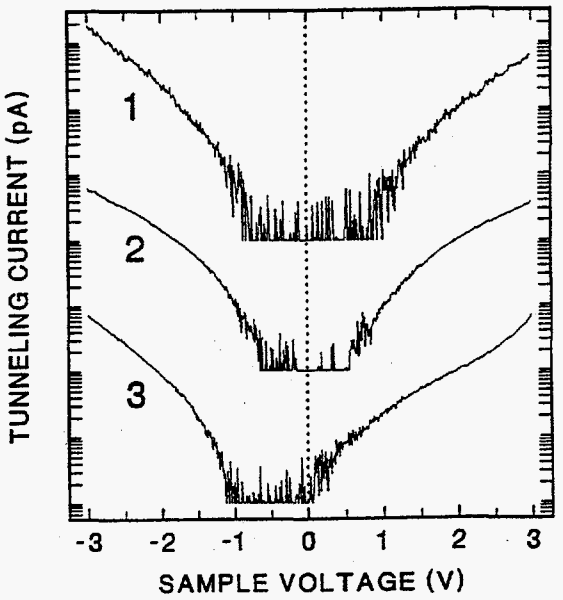

Fig. 1. Composition dependence of the insulating gap. The gap is wide (~1.8 eV) for $Sr_{0.3}Ca_{0.7}CuO_2$ (curve 1) and is expected to be undoped, but it is narrower for $SrCuO_2$ (curve 2), probably because of hole-doping Sr defects. Note the symmetric in-gap states for this composition. On the other hand, $Sr_{0.9}La_{0.1}CuO_2$ (curve 3), is electron-doped, producing in-gap states only at the bottom of the conduction band.

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1. Summary of paper to be published.
2. Osaka University, Osaka, Japan.

DEFECT FORMATION AND CARRIER DOPING IN EPITAXIAL FILMS OF THE INFINITE-LAYER COMPOUND[1]

R. Feenstra, S. J. Pennycook, M. F. Chisholm, N. D. Browning,[2] J. D. Budai, D. P. Norton, E. C. Jones,[3] D. K. Christen, T. Matsumoto,[4] and T. Kawai[4]

The infinite-layer compound $Sr_{1-x}A_xCuO_2$ represents the fundamental building block of the high-temperature superconductor (HTSc) copper-oxides. Thus, it provides the ultimate starting point for a systematic search for new materials, as well as basic studies of underlying mechanisms. The correlation between defect formation and carrier doping in epitaxial films of the end member $SrCuO_2$, which has the simplest chemistry of all infinite-layer compositions, has been studied. The materials were produced by molecular beam epitaxy (MBE) controlled layer-by-layer growth experiments, and the correlations were studied using a variety of complementary techniques—chemically resolved scanning transmission electron microscopy (*Z*-contrast STEM), scanning tunneling microscopy, x-ray diffraction, electrical transport measurements, and post-growth oxidation-reduction experiments.

Based on the combined information provided by these experiments, it is concluded that the carrier doping is dominated by the formation of an electron-doped matrix under mildly oxidizing growth conditions. This effect is augmented by metastability-induced tendencies for defect formation. Because of the lightly doped character of this parent-like compound, these defects can have a large effect on the electrical properties. High densities of planar defects perpendicular to the CuO_2 planes were observed in plan-view *Z*-contrast STEM images, suggesting mechanisms for the accommodation of local deviations in the stoichiometry. Superconductivity with $T_c \cong$ 25–45 K has been induced after high-temperature oxidation of films deliberately grown with excess Sr(O) monolayers in the basic structure, controlled through the MBE process.

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1. Summary of paper: p. 228 in *SPIE Conference on Oxide Superconductor Physics and Nano-Engineering II*, ed. by I. Bozovic and D. Pavuna, SPIE, Bellingham, Washington, 1996
2. University of Illinois, Urbana, Illinois.
3. Fusion Energy Division, ORNL.

Thin-Film Batteries and Solid Electrolytes

ORIENTED $LiCoO_2$ FILMS AND HIGH-RATE THIN-FILM LITHIUM BATTERIES[1]

J. B. Bates and N. J. Dudney

Crystalline $LiCoO_2$ has a layered structure in which the lithium and cobalt ions are located in alternate planes that are separated by closed-packed oxygen layers. Thin-film rechargeable lithium batteries with crystalline $LiCoO_2$ cathodes have high energy and power densities and can be cycled thousands of times with negligible capacity losses. In the diffraction patterns of the $LiCoO_2$ films measured after crystallization and prior to battery fabrication, the (003), (101), and (104) reflections are free from strong interfering peaks because of the alumina substrate and Pt current collector. The relative intensities of these reflections depend on the process parameters and, to a lesser extent, on subtle differences in the $LiCoO_2$ targets.

The $LiCoO_2$ films can be categorized into three types according to the relative integrated intensities of the (003), (101), and (104) reflections (Table 1). Comparing the film intensities with those of a (random) powdered sample of $LiCoO_2$ shows that the films exhibit strong texturing. The percentages of grains with their (003), (101), or (104) planes parallel to the substrate for the three types of films (Table 1) were calculated using the respective intensities for the films and the powder sample. Because lithium diffusion through the grains is fast along the ⟨101⟩ and ⟨104⟩ directions but is negligible along the ⟨003⟩ direction, batteries with cathodes of Type B and Type C can sustain much higher currents (~3×) than batteries with Type A cathodes having a 10% or larger percentage of (003) grains. This is illustrated in Fig. 1 which shows the graphs of capacity delivered between 4.2 and 3.0 V vs. current density for batteries with Type B and Type A cathodes of comparable thickness. Continuing research is focused on understanding the conditions which control the texture of sputter-deposited $LiCoO_2$ films.

Table 1. Relative x-ray intensities and percentage of grains with (003), (101), and (104) orientation.

Type	003	101	104
	Relative Intensity		
A	85	100	20
B	0	15	100
C	0	100	70
Powder	100	30	62
	Percentage		
A	19	74	7
B	0	24	76
C	0	75	25
Powder	33	33	33

1. Summary of paper to be published.

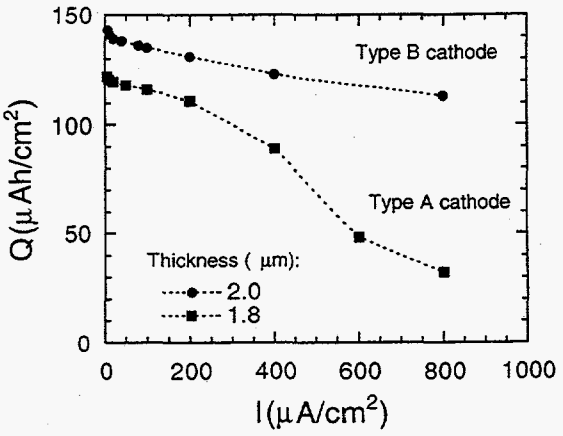

Fig. 1. Discharge capacity vs. current density.

AMORPHOUS $Li_xMn_{2-y}O_4$ CATHODES FOR THIN-FILM BATTERIES[1]

N. J. Dudney, J. B. Bates, R. A. Zuhr, J. D. Robertson[2]

Thin-film cathodes fabricated by sputter deposition from sintered or hot-pressed targets of $LiMn_2O_4$ consistently have high specific capacities and long cycle life. These cathodes have a density ~4.2 g/cm^3 and are amorphous by x-ray diffraction. The fracture cross section of Fig. 1 shows the columnar microstructure and good adhesion of this cathode with both the Ni current collector and the Lipon electrolyte films. Recent work has focused on the 6× film-to-film variation in the cathode resistivity which has been found to correlate roughly with the initial open-circuit voltage of the battery and also the sputter history of the target.

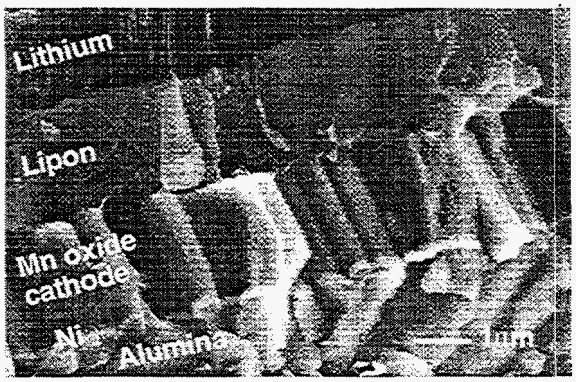

Fig. 1. Fracture cross section of a thin-film battery tested for over 6 mos at 25–100°C.

Analytical (Rutherford backscattering spectroscopy, proton-induced gamma emission spectroscopy, and inductively coupled plasma atomic spectroscopy) results of films deposited from targets with extreme differences in their sputter history give atomic ratios for O/Mn of 1.9–2.6 and Li/Mn of 0.5–1.25. These values are much larger than expected from the $LiMn_2O_4$ target composition. No detectable carbonate or hydroxide species, which might account for the high O/Mn, were found by IR spectroscopy, even after prolonged exposure of the films to air. The tendency for the film composition to vary with the sputter history of the target, often resulting in a Mn-deficient film, may be due to the diffusive Li redistribution within the $LiMn_2O_4$ sputter target.

The wide variation in composition is consistent with observed cycling results if the discharge behavior between 4.5 and 1.8 V reflects the Mn valence change from +4 to +3, regardless of the Li concentration. Although the film compositions may differ greatly [e.g., $Li_xMn_2O_4$ $(0 < x < 2)$ vs. $Li_xMn_{1.6}O_4$ $(1.6 < x < 3.2)$], the specific capacities for the Mn^{+4} to Mn^{+3} range, 27 5± 21 μAh/mg, are within the experimental uncertainty for our thin-film cathodes. The cathode resistivity, however, is more sensitive to the film composition. The resistivity is significantly smaller for films with a high initial open-circuit voltage, indicating that the Mn valence in the as-deposited films must be >3.5.

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1. Summary of paper to be published.
2. University of Kentucky, Lexington, Ky.

HYSTERESIS IN THE LITHIUM INSERTION REACTION OF AMORPHOUS CATHODES[1]

N. J. Dudney, J. B. Bates and F. X. Hart[2]

Thin-film rechargeable lithium batteries are based upon the reversible insertion reaction of lithium into the oxide cathode materials. A hysteresis in this reaction is apparent when cycling batteries with an amorphous Mn or V oxide cathode. Extensive temperature and equilibration-rate studies demonstrate that this is a true hysteresis, not a slow equilibration process. Similar hysteresis effects have been reported for bulk forms of amorphous or poorly crystalline cathode materials.

The so-called "scanning" curves[3] for the cycling of a thin-film battery with an amorphous cathode are shown in Fig. 1. Typical of a hysteresis, the lithium content in the cathode at a particular cell voltage (i.e., a particular chemical potential) depends on the charge/discharge path taken to equilibrate the cell. Most work in the literature relates this scanning behavior to domains in the material which have a distribution of thresholds impeding a first-order phase transformation. The barrier to the transformation might be due to such irreversible processes as the motion of boundaries, formation of dislocations, nucleation, plastic deformation, or disorder of the material.

A plausible model was constructed for the $Li_xMn_{2-y}O_4$ cathode based on a transformation between two phases in the 4.5 –3.0-V cycling range. This is illustrated by the free energy diagram in Fig. 2. Small energy barriers for the $\alpha \leftrightarrow \beta$ transformation shift the phase boundaries and the activity of lithium for the two-phase region creating a hysteresis loop. Experimentally, the energy dissipated for the lithium insertion reaction is ~4 kJ/mole. Identification of the α,β phases and the structural basis for the hysteresis are unknown.

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1. Summary of paper to be published.
2. University of the South, Sewanee, Tenn.
3. T. B. Flanagan e. al., *Prog. Solid State Chem.* **23** , 291 (1995).

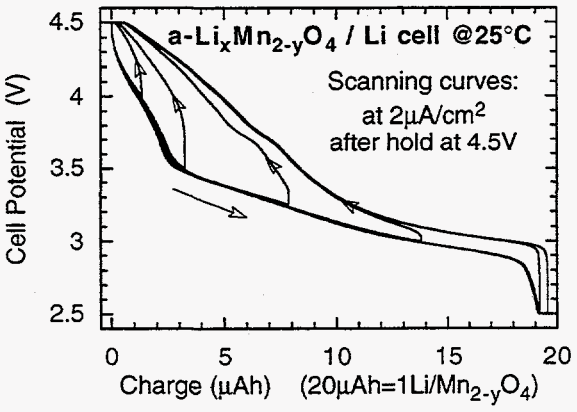

Fig. 1. Discharge-charge of thin-film battery.

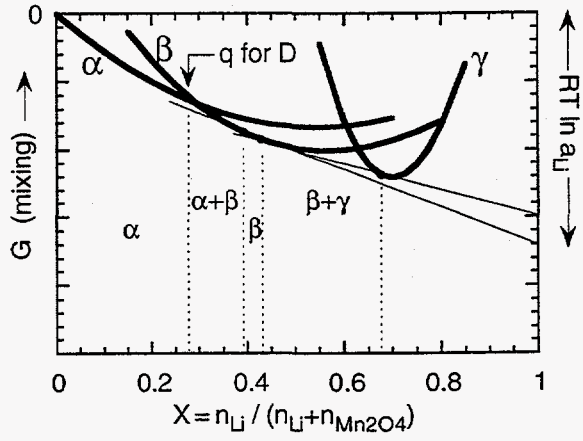

Fig. 2. Model of free energy for three Li-Mn_2O_4 phases showing threshold energy for discharge.

ELECTROCHEMICAL PROPERTIES AND DEFECT MODEL OF CRYSTALLINE $LiMn_2O_4$ THIN FILMS[1]

A. Ueda[2] and J. B. Bates

The structural and electrochemical properties of crystalline $LiMn_2O_4$ films depend on the deposition and annealing conditions. Films were deposited over Pt current collectors on alumina substrates by rf magnetron sputtering of $LiMn_2O_4$ in Ar + 10 % N_2 gas mixtures and annealed at 400° to 900°C in flowing O_2. From x-ray diffraction measurements, these films exhibited a cubic spinel structure with an *a*-axis length (a) that increased linearly with annealing temperature from 8.13 to 8.21 Å.

Cells with cathodes having different a values exhibit marked differences in the capacities at 3, 4, and 5 V, as illustrated in Fig. 1. In particular, the ratios of capacities at 4 and 3 V increase with a, as shown in Fig. 2. This behavior and the origin of the plateau at 5 V (Fig. 1) can be explained with a defect model represented by $[Li_{1-y}Mn_y]_{8a}[Li_xMn_{2-x}]_{16d}O_4$ where Li and Mn ions are located on tetrahedral 8a (Mn^{2+}) sites and octahedral 16d sites (Mn^{4+}, Mn^{3+}). The 3-V region results from the insertion of 1 Li^+ per 4 O^{2-} ions onto 16c sites accompanied by the reduction of an equal number of Mn^{4+} to Mn^{3+}. In the 4-V region, all of the 1–3 $x + y$ Mn^{3+} ions are oxidized to Mn^{4+} as 1–3 $x - y$ Li^+ ions are extracted from the 8a sites. It is speculated that the 5-V plateau arises from the extraction of the remaining $4x - 3y - 2$ Li^+ from the 8a sites accompanied by the oxidation of the Mn^{2+} ions on these sites. Using bulk data for the 4V/3V capacity ratio vs. a, the defect model qualitatively fits the thin-film data as shown by the solid curve in Fig. 2.

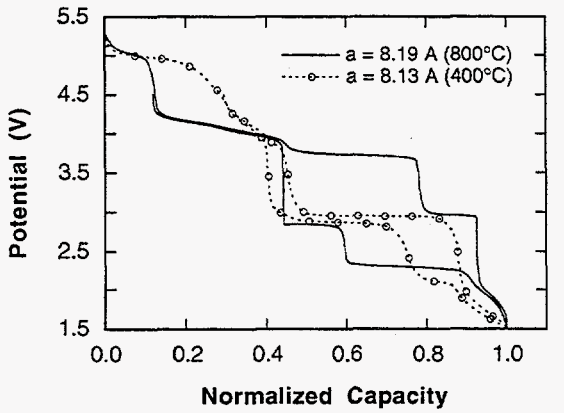

Fig. 1. Low-current discharge-charge curves for Li-$LiMn_2O_4$ cells with cathodes annealed at 400° and 800°C.

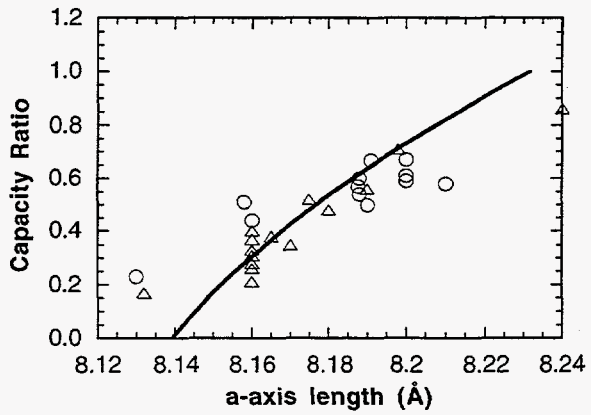

Fig. 2. Measured capacity ratios vs. a-axis length. The solid curve was calculated from a fit of the model bulk data for a vs. x in the model $Li[Li_xMn_{2-x}]O_4$.

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1. Summary of paper to be published.
2. ORNL/ORISE postdoctoral research associate.

MANGANESE-SUBSTITUTED LITHIUM NICKEL OXIDE $Li_xM_{2-x}O_2$ ($M = Mn_yNi_{1-y}$) THIN FILMS[1]

B. J. Neudecker,[2] R. A. Zuhr, B. S. Kwak,[3] J. D. Robertson,[4] and J. B. Bates

In view of high discharge capacities at high voltages, $LiNiO_2$ has gained much attention as a promising cathode material for rechargeable lithium batteries. However, a slight deviation from the ideal starting stoichiometry $LiNiO_2$ severely diminishes the electrochemical performance. The nickel migration into lithium vacancies, which occurs at charge voltages above 4.2 V, further lowers the reversible discharge capacity. For these reasons, manganese was substituted for nickel which, based on theoretical considerations, was expected to avoid some of the inherent drawbacks of the Li_xNiO_2 cathode.

Thin-film and bulk samples of the series $Li_x(Mn_yNi_{1-y})_{2-x}O_2$ were prepared by magnetron sputtering or solid state reactions, respectively, and their physical and electrochemical properties were thoroughly studied. The resulting phases were closely related to the phases of the parent series $Li_xNi_{2-x}O_2$ where $x \leq 1.33$.

Preparation conditions were established for virtually any x-value in the series $Li_x(Mn_yNi_{1-y})_{2-x}O_2$, where $y \leq 0.5$. From a comparison with the parent series $Li_xNi_{2-x}O_2$, the stoichiometric parameter x for $x \leq 1.33$ and $0.38 \leq y \geq 0.5$ can be accurately calculated from the x-ray density $\rho = (-1.920x + 6.549)$ g/cm^3 thus providing a powerful tool for determining the stoichiometry, which otherwise would require extensive ion beam analysis.

The electrochemical measurements suggest that a limited number of Ni^{3+} ions migrate from the 3a to the 3b sites as soon as more than 50% of the 3b sites ("lithium layers") become vacant on deintercalation. Nonetheless, $Li/Li_x(Mn_yNi_{1-y})_{2-x}O_2$ thin-film batteries, where $x > 1.0$, showed a high reversibility even when charged to 4.8 V (Fig. 1) or to 5.3 V. This is attributed to the appreciable amount of lithium ions remaining in the lithium layers even when manganese and nickel reach their maximum achievable electrochemical valence state of +4.

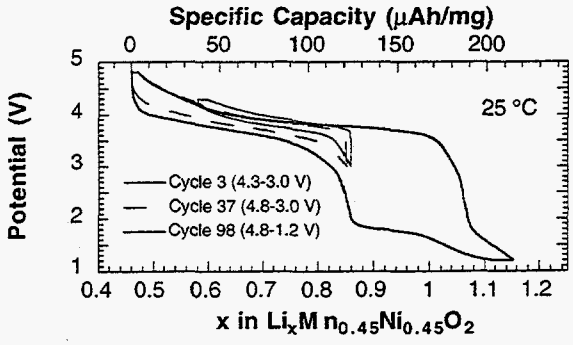

Fig. 1. The voltage profiles of a $Li/Li_xMn_{0.45}Ni_{0.45}O_2$ battery within different potential windows.

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1. Summary of paper to be published.
2. ORNL/ORISE postdoctoral research associate.
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4. University of Kentucky, Lexington, Ky.

IN SITU X-RAY DIFFRACTION MEASUREMENTS ON $LiMn_2O_4$ THIN FILMS IN Li-$LiMn_2O_4$ CELLS[1]

A. Ueda[2] and J. B. Bates

Cycling thin-film Li-$LiMn_2O_4$ cells between 5.3–1.2 V results in the exchange of 2.5 Li per Mn_2O_4. The effects of this large change in stoichiometry on the structure of $LiMn_2O_4$ was investigated by x-ray diffraction. Films of $LiMn_2O_4$ were fabricated as described elsewhere in this report[3] and incorporated into thin-film lithium cells. After depositing a protective coating over the cells, diffraction measurements were made at different equilibrium potentials.

The diffraction patterns observed in the region near the (111) reflection during a cycle from 4.5 to 1.2 to 5.3 V are shown in Fig. 1. On discharge from 4.5 V, the (111) peak shifts to smaller angles as lithium is inserted into the cathode. The sudden decrease[3] in cell voltage from 3.7 to 3 V signals the formation of a tetragonal phase which continues to grow at the expense of the spinel phase. As can be seen in Fig. 1, the intensity of the (101) peak of the tetragonal phase increases while the (111) spinel peak disappears. At the end of the 2-V plateau, the transformation is complete, and the potential decreases rapidly[3] as lithium is inserted into the (single) tetragonal phase. On the charge cycle, these transformations are reversed. However, the relative intensities of the (101) tetragonal and (111) spinel peaks are not the same at the corresponding potentials on discharge and charge. This is caused by a retardation in the rate of conversion of the minority phase as the transformation progresses in either direction. As the potential is increased from 4.5 to 5.3 V, all of the lithium is extracted from the lattice accompanied by what is believed to be a migration of Mn ions from tetrahedral to octahedral sites. Because no new peaks were observed in any accessible region of the diffraction patterns on following cycles, charging to 5.3 V evidently does not cause an irreversible change in the cathode structure.

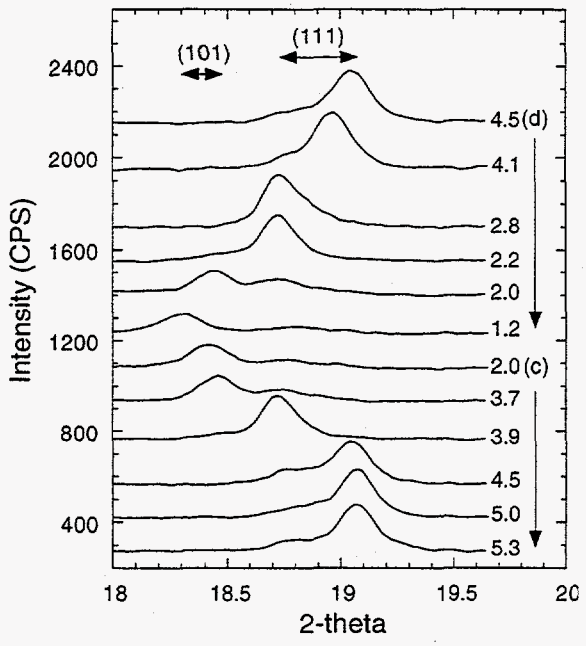

Fig. 1. X-ray measurements at selected potentials. The cell was discharged from 4.5 to 1.2 V and then charged to 5.3 V.

1. Summary of paper to published.
2. ORNL/ORISE postdoctoral research associate.
3. A. Ueda and J. B. Bates, "Electrochemical Properties and Defect Model of Crystalline $LiMn_2O_4$ Thin Films," this report.

ENHANCED DEPOSITION RATE OF LITHIUM PHOSPHORUS OXYNITRIDE THIN FILMS BY SPUTTERING OF Li_3PO_4 IN N_2-He GAS MIXTURES[1]

J. B. Bates and X. Yu[2]

The electrolyte in the ORNL-developed thin-film lithium batteries, lithium phosphorus oxynitride ("Lipon"), is usually deposited by rf magnetron sputtering of Li_3PO_4 in pure N_2. By sputtering in mixtures of N_2 and He, it was observed that the deposition rate is increased by as much as 50% in some cases for the same applied rf power.

Sputtering depends on the presence of positive ions in the plasma. The only positive species identified in the emission spectra (800–300 nm) during sputtering were N ions. In Fig. 1, the intensities of the three lines identified as vibronic transitions of N can be seen to increase with increasing He in the process gas. This is a result of Penning ionization, $N_2 + He^* = N + He + e$, where He* is an excited helium atom.

The intensity ratio, $I_r = I[N/I[N_2(0,3)]$, is a qualitative measure of the number of N ions in the plasma relative to the number of N_2 molecules. As shown in Fig. 2, the increase in rate follows the increase in I_r up to about 83% He where it decreases rapidly. As shown in Fig. 3, the function $[He][N_2]I_r$, where $[He] + [N_2] = 1$, mimics this behavior .

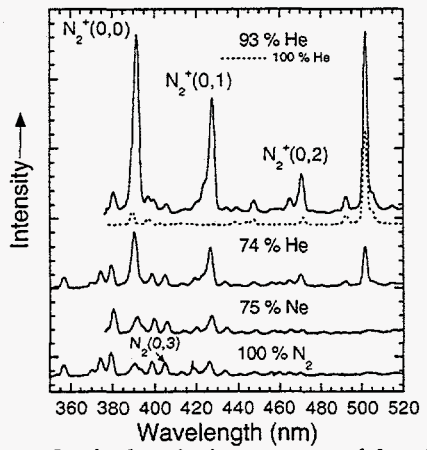

Fig. 1. Optical emission spectra of the plasma for different process gases.

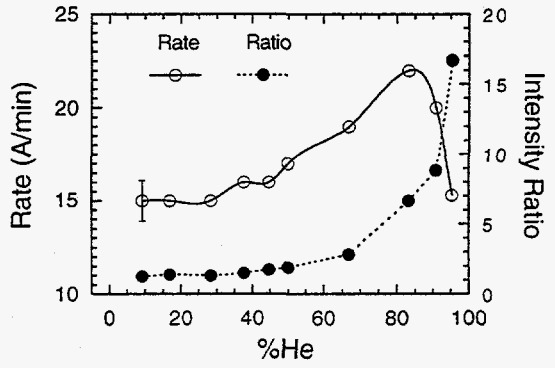

Fig. 2. Deposition rate and ratio of emission line intensities, $I[N]/I[N_2(0,3)]$ as a function of %He in the process gas.

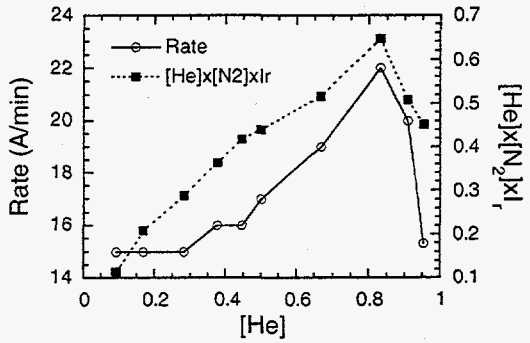

Fig. 3. Graphs of deposition rate and $[He][N_2]I_r$ vs. fraction of He in the process gas.

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1. Summary of paper: J. B. Bates and X. Yu, *J. Vac. Sci. and Technol. A* **14**, 34 (1996).
2. ORNL/ORISE postdoctoral research associate. Present address: Liebert Corporation, Columbus, Ohio.

Materials Development and Properties

NOVEL THERMOELECTRIC MATERIALS[1]

B. C. Sales

Several new approaches to the design of improved thermoelectric materials have stimulated a resurgence of interest in this very old field. Within the past several years, materials that validated one or more of these new ideas have been developed. Perhaps the most significant development is the concept and realization of materials that conduct electricity like a crystalline solid but conduct heat like a glass. In these materials, a weakly bound atom or molecule "rattler" is used to lower the thermal conductivity of the solid without severely affecting electronic conduction, thus leading to improved thermoelectric efficiency.

The major goal of thermoelectric materials research is to design materials that will improve the efficiency of solid state generators and refrigerators. Efficiency depends on material properties through the dimensionless figure of merit ZT, where T is the absolute temperature and $Z = S^2/kr$, where S is the thermopower or Seebeck coefficient, r is the electrical resistivity, and k is the total thermal conductivity. The total thermal conductivity can be broken into two parts $k = k_{electronic} + k_{lattice}$ where $k_{electronic}$ describes the heat conducted by the electrons (or holes) and $k_{lattice}$ the heat conducted by the crystalline lattice. For a particular device, the larger the value of ZT the higher the efficiency. Therefore, the goal of materials science is to find materials with the highest possible value of ZT. Current technology uses materials with ZT values near 1, but theory indicates that ZT values of 3 or 4 should be possible.

Three new approaches to improved thermoelectric materials are being investigated: rattling semiconductors, correlated metals and semiconductors (Fig. 1), and superlattices. All three approaches have resulted in the development of interesting new materials with unusual electronic or thermal properties. It should be noted, however, that none of the new materials discovered to date are any threat to replace the materials used in existing commercial thermoelectric devices.

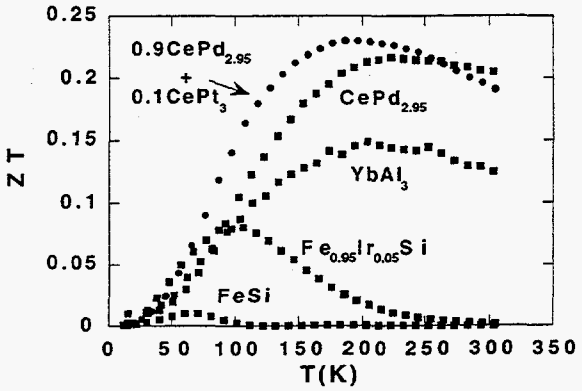

Fig. 1. ZT vs. temperature for several correlated metals and the correlated semiconductor FeSi.

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1. Summary of paper: *Current Opinion in Solid State Physics* (in press).

FILLED SKUTTERUDITE ANTIMONIDES: A NEW CLASS OF THERMOELECTRIC MATERIALS[1]

B. C. Sales, D. Mandrus, and R. K. Williams[2]

A new class of thermoelectric materials has been synthesized with a thermoelectric figure of merit (ZT) greater than 1 at 800 K. Although these new materials have not been optimized, this value for ZT is comparable to the best obtained on any previously studied thermoelectric material. Calculations (Fig. 1) indicate that optimized material should have ZT values of 1.4. These new ternary semiconductors have the general formula RM_4X_{12} and represent a new approach to creating improved thermoelectric materials. Several alloys in the composition range $AFe_{4-x}Co_xSb_{12}$ (A = La, Ce and $0 < x < 4$) have large values of ZT.

It has been proposed that the ultimate thermoelectric material should conduct electricity like a crystal but conduct heat like a glass. To find such a material, crystal structures containing weakly bound atoms or molecules that "rattle" within an atomic cage should be investigated. Since good electrical properties must be maintained, it is likely that there should be at least three distinct crystallographic sites in the structure (i.e., a true ternary compound). Two of the sites would form the basic framework of the structure, and this framework would dominate the band structure and, therefore, electronic transport. The third cage-like site would be occupied by the rattling atom that scatters the heat-carrying phonons, thus greatly reducing the lattice portion of the thermal conductivity. In the filled skutterudites, the rare-earth atom is the rattler, and good electronic conduction is maintained through the Sb and transition-metal orbitals.

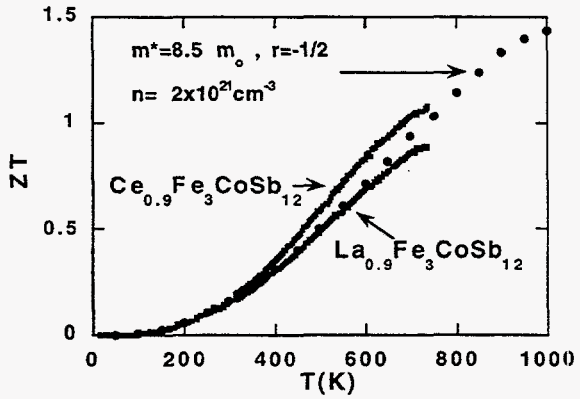

Fig. 1. ZT vs. temperature for nearly optimized samples of $La_{0.9}Fe_3CoSb_{12}$ and $Ce_{0.9}Fe_3CoSb_{12}$ (experimental data, squares). The values for ZT at higher temperatures were calculated (circles) using a single parabolic band, the assumption of scattering by acoustic phonons, and measured room-temperature values for the carrier concentration, Seebeck coefficient, and electrical conductivity. The measured high-temperature thermal conductivity was also used in the calculation.

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1. Summary of paper: *Science* **272**, 1325 (1996).
2. Metals and Ceramics Division, ORNL.

FILLED SKUTTERUDITE ANTIMONIDES: VALIDATION OF THE ELECTRON-CRYSTAL PHONON-GLASS APPROACH TO NEW THERMOELECTRIC MATERIALS[1]

D. Mandrus, B. C. Sales, V. Keppens,[2] B. C. Chakoumakos, P. Dai, L. A. Boatner, R. K. Williams,[3] J. R. Thompson,[4] T. W. Darling,[5] A. Migliori,[5] M. B. Maple,[6] D. A. Gajewski,[6] and E. J. Freeman[6]

One of the most promising new ideas in the field of thermoelectrics is the electron-crystal, phonon glass (ECPG) concept originally proposed by Slack.[7] In this picture, a loosely bound atom with a large thermal parameter scatters phonons much more strongly than electrons, thus permitting a "glasslike" thermal conductivity to coexist with the high electron mobilities found in crystals. A low thermal conductivity is desirable in a thermoelectric material because the maximum efficiency of a device built using such a material is related to the figure of merit $ZT = S^2\sigma T\kappa^{-1}$. Here S is the Seebeck coefficient, σ is the electrical conductivity, κ is the thermal conductivity, and T is the absolute temperature.

Very recently, Sales, Mandrus, and Williams[8] reported a high ZT in the filled skutterudite $LaFe_3CoSb_{12}$, which was primarily due to a drastic reduction in the lattice component of the thermal conductivity of this material compared with its unfilled analogue Co_4Sb_{12}. In the filled material, two La ions per unit cell occupy two large "holes" in the crystal structure. These La ions are weakly bound, have a large thermal parameter, and appear to undergo localized, incoherent vibrations.

The lattice dynamics of $LaFe_3CoSb_{12}$ have been studied using specific heat, resonant ultrasound spectroscopy (RUS), and inelastic neutron scattering (Fig. 1). The measurements reveal the existence of two low-energy vibrational modes in $LaFe_3CoSb_{12}$. It is likely that at least one of these modes represents the localized, incoherent vibrations of the La ion in its oversized atomic "cage." These results support the usefulness of weakly bound, "rattling" ions for the improvement of thermoelectric performance.

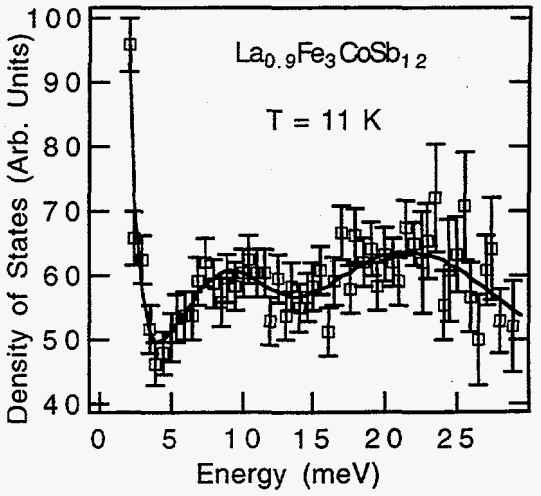

Fig. 1. Phonon density of states for $La_{0.9}Fe_3CoSb_{12}$ obtained using inelastic neutron scattering.

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1. Summary of Paper: *Materials Research Society Symposium Proceedings* **478** (in press).
2. ORNL/ORISE postdoctoral research associate.
3. Metals and Ceramics Division, ORNL.
4. Adjunct R&D participant from The University of Tennessee, Knoxville, Tenn.
5. Los Alamos National Laboratory, Los Alamos, N. Mex.
6. University of California, San Diego, La Jolla, Calif.
7. G. A. Slack, p. 407 in *The CRC Handbook of Thermoelectrics*, ed. by D. M. Rowe, CRC Press, Boca Raton, Fla., 1995.
8. B. C. Sales, D. Mandrus, and R. K. Williams, *Science* **272**, 1325 (1996).

OPTICAL SWITCHING OF COHERENT VO_2 PRECIPITATES FORMED IN SAPPHIRE BY ION IMPLANTATION AND ANNEALING[1]

L. A. Gea[2] and L. A. Boatner

Substances in which both sensing and actuating functions are coupled by an intrinsic control mechanism are known as "smart" materials. The intriguing basic properties of these materials and their potential for applications have recently provided the motivation for a number of research activities.

The case of thin films of VO_2 deposited on various substrates is a classic example of a smart surface. VO_2 undergoes a first-order monoclinic-to-tetragonal (and semiconducting-to-metallic) phase transition at ~68°C. When VO_2 films are illuminated with intense laser light, the resulting temperature increase can induce a rapid (>5 ps) semiconducting-to-metal phase transformation. The metallic VO_2 phase then produces a reflecting surface that strongly attenuates further transmission of the incident radiation. Thus, the VO_2 film performs both sensing and actuating functions through coupled intrinsic properties.

A new type of precipitate/host-composite surface has been formed by ion implantation and thermal annealing. Precipitates of VO_2 that are "embedded" in a sapphire substrate and that produce an optically active surface by exploiting the semiconducting-to-metal VO_2 phase transition are formed. One advantage of this composite surface is that the precipitates are an integral part of the near surface of the host and are protected from the environment.

Since the optical properties of VO_2 change dramatically at the transition, the formation of the VO_2 phase by means of implantation and annealing was established using optical-transmission measurements. Figure 1 shows the results of an optical measurement made at a wavelength of 3.4 μm as the temperature of the specimen was scanned between 320 and 365 K. The top trace shows the transmission curve obtained by heating and cooling the sample at a rate of 2°C/min. This implantation and annealing approach can be applied to form other systems by combining different "active" precipitates with various host lattices.

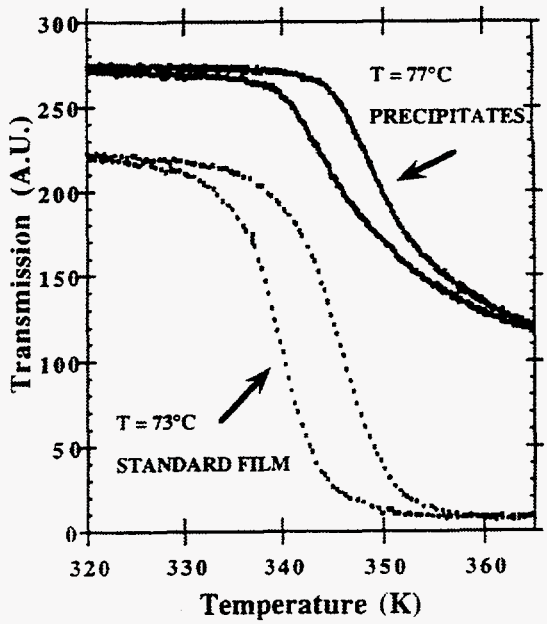

Fig. 1. Optical transmission spectrum at 3.4 μm showing the hysteretic VO_2 phase transition for: (a) VO_2 precipitates in Al_2O_3 coimplanted with V and O and annealed (top: T_c ~ 77°Ç) and (b) a thin film of VO_2 deposited on Al_2O_3 (bottom: T_c ~ 73°C).

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1. Summary of paper: *Appl. Phys. Lett.* **68**, 3081 (1996).

2. ORNL/ORISE postdoctoral research associate.

THE GROWTH AND PROPERTIES OF EPITAXIAL $KNbO_3$ THIN FILMS AND $KNbO_3/KTaO_3$ SUPERLATTICES[1]

H.-M. Christen,[2] L. A. Boatner, J. D. Budai, M. F. Chisholm, L. A. Gea,[3] P. J. Marrero,[4] and D. P. Norton

The ferroelectric properties in perovskites can be drastically altered by small structural changes introduced either through defect-induced distortions or by external mechanical stresses. In the first case, a random substitution of one ion for another of a slightly different ionic radius may result in ferroelectric or "glassy" polar states. For externally applied stress, possibilities for inducing changes in a bulk sample are somewhat limited, but surface tension can lead to a loss of ferroelectricity in fine-grained ceramics.

Heterostructures of alternating para- and ferroelectric thin films offer an interesting alternative. A superlattice in which one of the two materials changes its structure due to the "clamping" effect of the neighboring films may exhibit novel properties. Additionally, if a given ferroelectric structure exists over a range of film thicknesses, then size effects in ferroelectrics can be studied without being masked by depolarization fields.

A superlattice system of alternating paraelectric $KTaO_3$ and ferroelectric $KNbO_3$ layers, with excellent crystalline quality and a lattice mismatch below 0.5% by pulsed-laser deposition, has been grown. These thin-film structures were analyzed by Rutherford backscattering/ion channeling techniques, x-ray θ-2θ and Φ scans, and both conventional and Z-contrast scanning transmission electron microscopy. Figure 1 shows the θ-2θ x-ray scan for a single $KNbO_3$ film grown on (001)-oriented $KTaO_3$. The inset of Fig. 1 shows an expanded view of the (002) reflection where the interference pattern demonstrates the flatness of the film. A rocking curve across the same reflection shows a very small mosaic spread of about 0.05°.

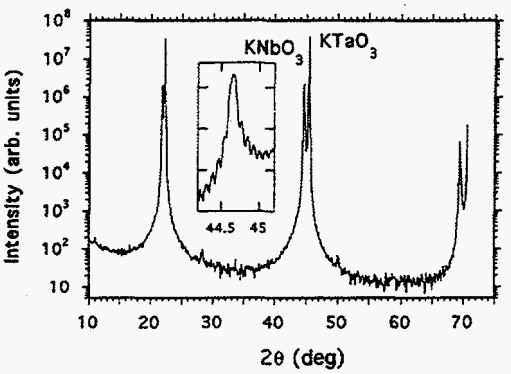

Fig. 1. X-ray θ-2θ scan along the substrate surface normal for a $KNbO_3$ film on $KTaO_3$. The inset shows an expanded view of the (002) film reflection with the interference pattern demonstrating the flatness of the film

With the excellent lattice match between these two materials, it should be possible to study size effects on the polar behavior of the dielectric properties of $KNbO_3/KTaO_3$ superlattice structures by growing samples on conducting substrates and to distinguish between true "size effects" in these structures and the influence of strains.

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1. Summary of paper: *Appl. Phys. Lett.* 68, 1488 (1996).
2. ORNL/ORISE postdoctoral research associate. Present address: Neocera, Inc., Beltsville, Md.
3. ORNL/ORISE postdoctoral research associate.
4. Universidad de Puerto Rico, Mayaguez, Puerto Rico.

PULSED-LASER DEPOSITION OF SOLID-SOLUTION FILMS USING SEGMENTED TARGETS[1]

H.-M. Christen,[2] D. P. Norton, L. A. Gea,[3] and L. A. Boatner

Many solid-solution systems exhibit physical and electronic properties that can readily be controlled by adjusting the ratio of the constituents. A new method for growing solid-solution thin films, where the ratio of the solid-solution components can be predetermined and varied over a wide compositional range, has been developed and applied to the case of the ferroelectric solid solution $KTa_{1-x}Nb_xO_3$ (KTN). The interest in KTN in bulk and thin-film forms has its origins in the large dielectric permittivity and electro-optic effects exhibited by this material at temperatures near the ferroelectric Curie point T_c. By adjusting the Ta/Nb ratio in the solid solution, the paraelectric/ferroelectric transition temperature can be varied continuously from 0 K ($x \leq 0.008$) to 35°C (i.e., to the T_c for pure $KNbO_3$).

For the growth of solid-solution layers with varying Ta/Nb ratios, a series of KTN targets could be used, but the optimum sintering parameters would have to be determined for each ceramic. This difficulty is avoided by our new approach, which requires only $KTaO_3$ and $KNbO_3$ pellets, and where one segmented target can grow films of various Ta/Nb ratios. Hot-pressed $KTaO_3$ and $KNbO_3$ ceramics were cut into wedge-shaped segments and mounted to form a portion of the target shown in Fig. 1. A semicircular KNO_3 pellet compensated for the volatility of potassium. The segmented target was mounted so that the center of rotation could be displaced from the center of the target by a distance d. The laser was focused on the target at a distance R from the center of rotation, so that ablation took place in a circular pattern, shown in Fig. 1. In this approach, the fraction P_{nb} of laser shots fired into the $KNbO_3$ ceramic directly determines the composition of the final $KTa_{1-x}Nb_xO_3$ film, and the value of x can be calculated as:

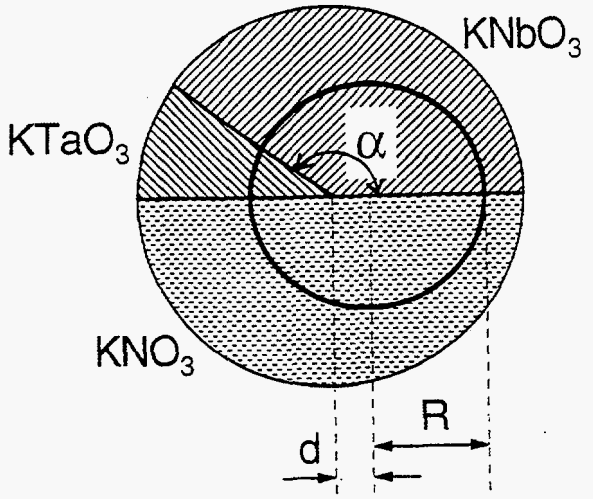

Fig. 1. Segmented target for the film growth of the solid solution between $KTaO_3$ and $KNbO_3$. The target is mounted on a rotating holder so that the center of rotation is displaced from the target center by a distance d. The laser is focused on a point at a distance R from the center of rotation,

$$x = P_{nb} = \frac{1}{x}\left\{\alpha + \arcsin\left(\frac{d}{R}\sin\alpha\right)\right\}$$

where α is the angle associated with the $KNbO_3$ wedge, as shown in Fig. 1.

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1. Summary of paper: *Thin Solid Films* (in press).
2. ORNL/ORISE postdoctoral research associate. Present address: Neocera, Inc., Beltsville, Md.
3. ORNL/ORISE postdoctoral research associate.

SEMICONDUCTING EPITAXIAL FILMS OF METASTABLE $SrRu_{0.5}Sn_{0.5}O_3$ GROWN BY PULSED-LASER DEPOSITION[1]

H.-M. Christen,[2] L. A. Boatner, J. D. Budai, M. F. Chisholm, L. A. Gea,[3] D. P. Norton, C. Gerber,[4] and M. Urbanik[5]

The development of crystalline conducting oxide films has recently received increased attention because of their importance in the formation of epitaxial heterostructures and devices that contain superconducting layers or ferroelectric films. Normal conducting oxide films provide the nontunneling weak links required in high-T_c superconductor Josephson junction applications.

Electrically conducting, lattice-matched "bottom" electrode films are required when electric fields are to be applied to overlying epitaxial thin-film structures. Recently, the cubic perovskite potassium tantalate ($KTaO_3$) has been used as a bulk substrate for the epitaxial growth of films of high-T_c superconductors, ferroelectrics, and metals; accordingly, the purpose of the present study was to develop new conducting films with a lattice constant matching that of $KTaO_3$.

The study of $SrRu_{0.5}Sn_{0.5}O_3$ was motivated by the successful use of $SrRuO_3$ in previous applications. While the lattice constant of $SrRuO_3$ can be reduced by substitution of calcium for strontium, replacing strontium with the larger Ba ion did not produce films with an increased unit cell. Rather than replacing Sr with larger ions, a substitution of larger ions for ruthenium was investigated.

Thin films of $SrRu_{0.5}Sn_{0.5}O_3$ were grown on (001) $KTaO_3$ single-crystal substrates by pulsed-laser deposition. These films exhibited a commensurate in-plane lattice match with $KTaO_3$ (a = 3.989 Å). $SrRu_{0.5}Sn_{0.5}O_3$ films were analyzed using x-ray diffraction, Rutherford backscattering, and atomic force microscopy. Figure 1 shows a θ-2θ scan across the substrate and film (002) reflections for a 600-nm-thick $SrRu_{0.5}Sn_{0.5}O_3$ layer deposited on $KTaO_3$.

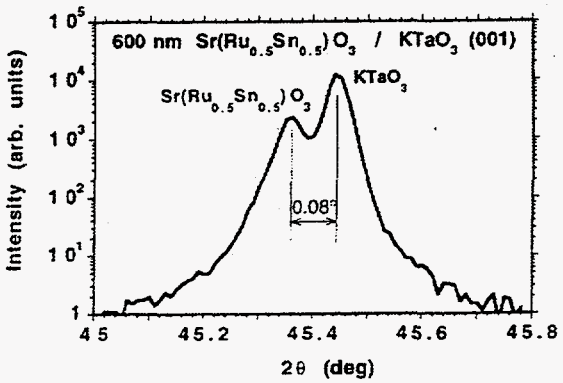

Fig. 1. X-ray θ-2θ scan for a 600-nm-thick $SrRu_{0.5}Sn_{0.5}O_3$ film on $KTaO_3$ (log scale). The substrate and film (002) reflections are visible.

$KTaO_3$ substrates coated with this new oxide should prove useful in thin-film studies of materials exhibiting properties that depend strongly on the lattice constant or on strains resulting from a "clamping" of the film to the substrate.

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1. Summary of papers: *Appl. Phys. Lett.* **70**, 2147 (1997); *Mat. Res. Soc. Symp. Proc.* **401**, 203 (1996).
2. ORNL/ORISE postdoctoral research associate. Present address: Neocera, Inc., Beltsville, Md..
3. ORNL/ORISE postdoctoral research associate.
4. IBM Research Division, Rüschlikon, Switzerland.
5. Commercial Crystal Laboratories, Inc., Naples, Fla.

SUBSTRATE DEPENDENCE IN THE GROWTH OF EPITAXIAL $Pb_{1-x}La_xTiO_3$ THIN FILMS[1]

Y. Kim,[2] A. Erbil,[2] and L. A. Boatner

In recent years, there has been a number of investigations dealing with the growth and properties of ferroelectric thin films. Thin films of the material $Pb_{1-x}La_xTiO_3$ (PLT) are of special interest because of the Lr excellent linear electro-optic, quadratic electro-optic, and pyroelectric properties. In many device applications of interest, thin films of PLT must be epitaxial to achieve low working voltages, low optical-propagation losses, and large electro-optic effects. The growth of even a single layer of a fully epitaxially oriented thin film of a complex-oxide like PLT is difficult.

In this work, the metalorganic chemical vapor deposition (MOCVD) technique has been applied to the growth of epitaxial PLT thin films with $x = 0.28$. The metalorganic precursors employed for each of the components were tetraethyl lead $[Pb(C_2H_5)_4]$, lanthanum B-diketonate $[La(C_{11}H_{19}O_2)_3]$, and titanium isopropoxide $[Ti(OC_3H_7)_4]$. Argon was the carrier gas.

For films deposited directly on (100) MgO substrates without an initial TiO_2 layer, a polycrystalline film was grown. However, by first introducing the titanium isopropoxide for a 20-s time period in order to grow an initial TiO_2 layer, it was possible to deposit three dimensionally epitaxial PLT films on MgO.

For both $KTaO_3$ and Al_2O_3 substrates, heteroepitaxy was achieved without the introduction of TiO_2 as the initial layer between the PLT film and the substrate. Figure 1 shows plots of the θ-2θ scan from 18° to 50° in 2θ for PLT thin films deposited on $KTaO_3$ (100) and Al_2O_3 (0001) substrates. Because of the isostructural nature of the $KTaO_3$ substrate and the PLT film and the good lattice match in this case, the diffraction peaks observed from the PLT (100) and (200) planes overlap those from the $KTaO_3$ (100) and (200) planes. PLT films with a [111]-preferred orientation were grown on the (0001)-oriented Al_2O_3 substrates, as expected. The rocking curves showed mosaic spreads with a full width at half maximum of about 0.30° and 0.25° for the films grown on MgO (100) and Al_2O_3 (0001) substrates, respectively.

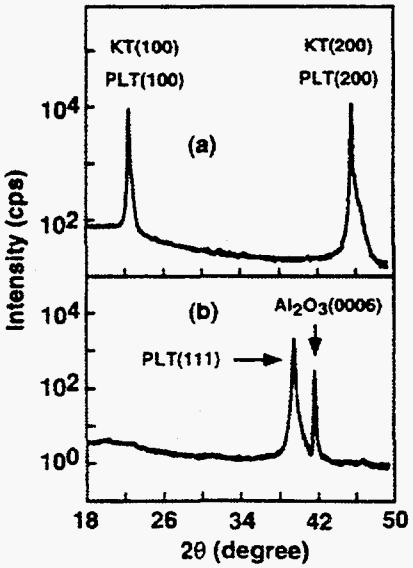

Fig. 1. θ-2θ x-ray diffraction patterns from PLT thin films grown on (a) $KTaO_3$ (100) and (b) Al_2O_3 (0001). The film thicknesses are 300 and 455 nm, respectively.

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1. Summary of paper: *Appl. Phys. Lett.* **69**, 2187 (1996).

2. Georgia Institute of Technology, Atlanta, Ga.

OPTICAL PROPERTIES OF EPITAXIAL $Pb_{1-x}La_xTiO_3$ THIN FILMS[1]

Y. Kim,[2] A. Erbil,[2] L. A. Boatner, L. Steingar,[3] T. Mensah,[4] and S. Hiamang[4]

Ferroelectric thin films are currently of general interest for fabricating novel devices. The ferroelectric $Pb_{1-x}La_xTiO_3$ (PLT) is a transparent material that results from the addition of La as a chemical modifier to $PbTiO_3$, and it is well known that PLT thin films have excellent quadratic electro-optic effects and a linear electro-optic effect for x values of 0.28 and 0.21, respectively. Because of these effects, PLT thin films are expected to be useful in the development of various optoelectronic devices. Applications involving optoelectronic devices based on optical waveguides require epitaxial PLT films with high transparency, and prior work on the preparation of PLT thin films has shown that PLT films possessing good optical properties can be prepared by rf-planar magnetron sputtering and rf-sputtering.

In the present work, metalorganic chemical vapor deposition (MOCVD) was used to prepare epitaxial or highly oriented PLT thin films with x values in the range 0.21–0.34. In all cases, the film deposition was carried out in an inverted vertical, warm-wall reactor vessel using a resistively heated susceptor. The crystallographic structure of the as-grown PLT thin films was examined by x-ray diffraction methods, and Rutherford backscattering (RBS) and RBS/channeling experiments were performed in order to determine the film thickness, composition, and crystallographic perfection. The refractive indices at different wavelengths were obtained by using a prism coupler with a rutile prism.

The MOCVD growth of PLT films resulted in three-dimensional epitaxial structures on the (100) surface of both MgO and $KTaO_3$ substrates. The films exhibited a single-phase perovskite structure with (100) planes parallel to the substrate surface. The PLT film grown on a $KTaO_3$ (100) substrate has a significantly lower minimum yield compared with that grown on an MgO (100) substrate because of the smaller lattice mismatch associated with $KTaO_3$. The thickness and refractive indices, which are in the wavelength range 435–1523 nm, were measured by the prism coupling method. The measured film thickness of 570 nm was in good agreement with that obtained from RBS measurements. The refractive index of the PLT film is smaller than that of $PbTiO_3$, and its difference at λ = 632.8 nm is about 2.5%. The dispersion of the refractive index was well fit by a Sellmeier dispersion formula. These results show that (100) $KTaO_3$ substrates provide an excellent lattice match for the growth of high-quality PLT epitaxial films.

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1. Summary of paper: *Mat. Res. Soc. Symp. Proc.* **401**, 267 (1996).
2. Georgia Institute of Technology, Atlanta, Ga.
3. Metricon Corporation, Pennington, N.J.
4. Clark Atlanta University, Atlanta, Ga.

ELECTRON-IRRADIATION-INDUCED NUCLEATION AND GROWTH IN AMORPHOUS $LaPO_4$, $ScPO_4$, AND ZIRCON[1]

A. Meldrum,[2] L. A. Boatner, and R. C. Ewing[2]

Electron-irradiation-induced annealing phenomena have been well documented in the case of amorphous metals and alloys, and they occur under a variety of conditions in semiconductors. Most of the previous work on electron-beam annealing of radiation damage has involved the epitaxial recrystallization of buried amorphous layers in Si because of the importance of this process in the semiconductor industry. The nucleation and growth of amorphous insulating materials under electron irradiation have only rarely been documented. Recently, however, electron irradiation has been shown to strongly inhibit the amorphization process during the heavy-particle irradiation of insulators.[3]

Here, synthetic $LaPO_4$, $ScPO_4$, and crystalline natural zircon ($ZrSiO_4$) from Australia were irradiated by 1.5-MeV Kr^+ ions until complete amorphization occurred, as indicated by the absence of electron-diffraction maxima. The resulting amorphous materials were irradiated by an 80- to 200-keV electron beam in the transmission electron microscope at temperatures between 130 and 800 K. The microstructural changes were monitored in situ. Thermal anneals in the range 500–600 K were also conducted to compare thermally induced microstructural development with that produced by electron irradiations.

Amorphous $LaPO_4$ and $ScPO_4$ annealed to form a randomly oriented polycrystalline assemblage of the same composition as the original material, but zircon recrystallized to ZrO_2 + amorphous SiO_2 for all beam energies and temperatures investigated. The rate of annealing increased in the order: zircon, $ScPO_4$, $LaPO_4$. Submicron tracks of crystallites having a width equal to that of the electron beam could be "drawn" on the amorphous substrate. In contrast, thermal annealing resulted in epitaxial recrystallization from the thick edges of the TEM samples.

Electron-beam-induced nucleation and growth in these materials can be explained by a combination of radiation-enhanced diffusion and a strong thermodynamic driving force for crystallization. The structure of the amorphous orthophosphates may be less rigid than that of their silicate analogues because of the lower coordination across the PO_4 tetrahedron, and thus, a lower energy is required for recrystallization. The more highly constrained monazite structure recovers at a lower electron dose than the zircon structure, consistent with a recent study of the crystalline-to-amorphous transition as a result of ion irradiation.

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1. Summary of paper: *Journal of Materials Research* (in press).
2. University of New Mexico, Albuquerque, N. Mex.
3. A. Meldrum et al., *Nuclear Instruments and Methods in Physics Research Section B* (in press).

DISPLACIVE RADIATION EFFECTS IN THE MONAZITE ZIRCON STRUCTURE ORTHOPHOSPHATES[1]

A. Meldrum,[2] L. A. Boatner, and R. C. Ewing[2]

The effects of displacive radiation on various ceramic materials continues to be extensively investigated—stimulated, in part, by current and potential future applications of ceramics in the nuclear industry (including their proposed use as "radiation-resistant" reactor materials or as single- or multi-phase crystalline nuclear waste forms). For example, $LaPO_4$ is currently under active investigation in Japan for the precipitation of actinides from nuclear waste tanks. The lanthanide orthophosphate series of compounds $LnPO_4$ (where Ln = La to Lu) encompasses materials with the monoclinic monazite structure as well as the tetragonal zircon structure, and this system provides an excellent model for the study of the susceptibility of ceramics to irradiation-induced amorphization.

In the present work, monazite-structure orthophosphates, including $LaPO_4$, $PrPO_4$, $NdPO_4$, $SmPO_4$, $EuPO_4$, $GdPO_4$, and natural monazite, and their zircon-structure analogues, including $ScPO_4$, YPO_4, $TbPO_4$, $TmPO_4$, $YbPO_4$, and $LuPO_4$, were irradiated by 800-keV Kr^{2+} ions in the temperature range 20–600 K. The critical amorphization dose was determined in situ as a function of temperature using selected-area electron diffraction. Amorphization doses were in the range 10^{14}–10^{16} ions/cm^2, depending on the temperature. Materials with the zircon structure were amorphized at higher temperatures than those with the monazite structure. The critical amorphization temperature ranged from 350 to 485 K for orthophosphates with the monazite structure and from 480 to 580 K for those with the zircon structure. Within each structure type, the critical temperature of amorphization increased with the atomic number of the lanthanide cation. Structural topology models are consistent with the observed differences between the two structure types but do not predict the relative amorphization doses for different compositions. The ratio of electronic- to-nuclear stopping correlates well with the observed sequence of susceptibility to amorphization within each structure type, consistent with previous results that electronic energy losses enhance defect recombination in the orthophosphates. The results clearly show that the monazite-structure orthophosphates have lower critical temperatures for amorphization than their zircon structure analogues and are, in general, more difficult to amorphize at $T > 300$ K.

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1. Summary of paper: *Physical Review B* (in press).

2. University of New Mexico, Albuquerque, N. Mex.

EXCITED STATE ABSORPTION AND FLUORESCENCE LINE NARROWING STUDIES OF Cm^{3+} IN $LuPO_4$[1]

K. M. Murdoch,[2] N. M. Edelstein,[2] L. A. Boatner, and M. M. Abraham[3]

Recently, a number of reports[4,5] have been published on the electron paramagnetic resonance (EPR) and optical spectra of Cm^{3+} ions in single-crystal $LuPO_4$. The Cm^{3+} ion replaces a Lu^{3+} ion at the D_{2d} symmetry site. In these earlier studies, $Cm^{3+}/LuPO_4$ crystal-field levels up to 34,000 cm^{-1} were measured by absorption spectroscopy and fitted to the parameters of an empirical Hamiltonian.

In the present work, laser-selective excitation spectroscopy was used to obtain additional experimental energy levels of the Cm^{3+} center. Its absorption transitions exhibited inhomogeneously broadened FWHM linewidths of ~2.3 cm^{-1}. This compares to an overall crystal-field splitting of the nominally $^8S_{7/2}$ ground state of 9.5 cm^{-1}. Fluorescence line narrowing (FLN) was used to resolve these ground-term splittings. In FLN experiments, the observed linewidths are limited by the either the bandwidth of the laser line or the resolution of the monochromator, so the energies of many of the levels found previously by absorption spectroscopy could be determined more accurately.

A single crystal of $LuPO_4$ doped with almost isotopically pure ^{248}Cm and grown using the flux technique described previously was used in the determination of crystal-field levels up to 35,700 cm^{-1} for the principal D_{2d} symmetry site. Eighty levels were assigned and fitted to a parametric Hamiltonian with an rms deviation of 28.4 cm^{-1}. Inhomogeneous broadening of the electronic transitions and the small 9.5-cm^{-1} splitting of the nominally $^8S_{7/2}$ ground multiplet are responsible for the satellite lines reported previously.

Subsites of the intrinsic Cm^{3+} center arise from the presence of defects and impurities in the $LuPO_4$ crystal. The electronic transitions were inhomogeneously broadened because the Cm^{3+} ions in different subsites experienced slightly different crystal fields. FLN spectra showed that the crystal-field splittings of the nominally $^8S_{7/2}$ multiplet differed by less than 0.1 cm^{-1} between subsites within these broadened transitions. The observed broadening was due to changes in the crystal-field splitting of the excited multiplets.

Energy transfer between the different subsites of the intrinsic Cm^{3+} center was observed by time-resolved fluorescence line narrowing (TRFLN). Sequences of TRFLN spectra were recorded and used to establish that electric-dipole interactions mediate this energy transfer. The transfer rate increased on warming the crystal above 4 K. This increase is indicative of the phonon-assisted energy-transfer-process. This is believed to be the first report of interion energy transfer in a Cm^{3+}-doped system.

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1. Summary of paper: *J. Chem. Phys.* **105**, 2359 (1996).
2. Lawrence Berkeley National Laboratory, Berkeley, Calif.
3. ORNL retiree.
4. W. K. Kot et al., *Phys. Rev. B* **48**, 12704 (1993)
5. J. Sytsma et al., *Phys. Rev. B* **52**, 12668 (1995).

ELECTRONIC STRUCTURE OF $ScPO_4$ SINGLE CRYSTALS: OPTICAL AND PHOTOELECTRIC PROPERTIES[1]

A. Trukhin[2] and L. A. Boatner

Experimental measurements have been made of the previously undetermined optical gap, band gap, and electronic structure of flux-grown single crystals of $ScPO_4$.

The $ScPO_4$ absorption spectra measured at the intrinsic absorption threshold corresponded well to the Urbach-Toyozawa Rule[3] for the case of strong exciton-phonon interactions. The expressions for the Urbach Rule are given by:

$$\alpha = \alpha_0 \exp[-\sigma(E_0 - E)/kT] \qquad (1)$$

$$\sigma = \sigma_0 2kT/\hbar\omega \tan(\hbar\omega/2kT) \qquad (2)$$

For the case of $ScPO_4$, the crossing point, E_0 = 7.75 ± 0.05 eV, was located below the maximum of the broad structureless absorption band at 8.8 eV whose position could be estimated from reflectivity spectra. The values of both the crossing point and of the parameter $\sigma_0 = 0.63$ corresponded to Toyozawa's criterion for a strong exciton-phonon in $ScPO_4$ because the Urbach's Rule parameters do not depend on impurities within the experimental error.

The self-trapped exciton (STE) luminescence band at 5.6 eV could be excited at energies of 7 eV and higher. This luminescence was strongly polarized (P = 70%) along the optical axes of the crystal, and the luminescence-decay time constant (τ) was about 1 ms near 4.2 K. The decay kinetics exhibit two ranges in which τ decreases strongly with increasing temperatures—a low-temperature range associated with the zero-field splitting of the STE triplet states and a second region where decreases in both τ and P arise from reorientations of the STE. The thermal-quenching energy of the STE luminescence is 0.22 eV with a rate of 5×10^5, and the reorientation activation energy is 0.02 eV with a rate of only 200.

The $ScPO_4$ energy gap of 7.2 eV at 293 K was determined using the data shown in Fig. 1, and the photoelectron emission threshold was estimated as ~8.5 eV for the direct transitions. The existing results show that the photoelectron emission takes place throughout the entire range of the intrinsic absorption.

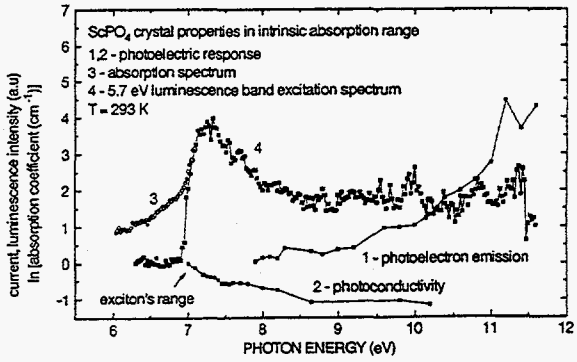

Fig. 1. Comparison of the optical absorption at the intrinsic edge, STE, luminescence excitation, and photoelectric response spectra in $ScPO_4$.

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1. Summary of paper: *Materials Science Forum* (in press).
2. University of Latvia, Riga, Latvia.
3. Y. A. Toyozawa, *Tech. Report ISSP* **A1**, 119 (1964).

SONOCHEMICAL SYNTHESIS OF $C_{60}H_2$[1]

D. Mandrus, M. Kele,[2] R. L. Hettich,[3] G. Guiochon,[4] B. C. Sales, and L. A. Boatner

Although acoustic cavitation (i.e., the sonically induced nucleation, growth, and implosive collapse of bubbles in a liquid) has been studied since the 1930s, it is only during the last decade that the chemical environment inside the collapsing bubbles has been successfully characterized. The sonochemical environment is a unique, high-energy environment. It has been found that the temperature and pressure inside the collapsing bubbles can exceed 5000 K and 1000 atm and that the associated cooling rate can exceed 10^9 K/s.[5] There is also evidence that the liquid itself, if injected into a bubble during collapse, can experience temperatures as high as 2000 K.[6]

$C_{60}H_2$ has been synthesized by ultrasonically irradiating solutions of C_{60} in decahydronaphthalene. Mass spectrometry, high-performance liquid chromatography, and UV-vis spectrophotometry were used to characterize the reaction products. The synthesis of $C_{60}H_2$ can be understood as a secondary reaction arising from the production of atomic hydrogen during sonolysis of the solvent. Continued sonication results in both the disappearance of C_{60} and $C_{60}H_2$ from the solution and the formation of a novel C_{60}-based polymeric material. These data suggest that the C_{60} experiences a high-energy environment during ultrasonic irradiation that can be exploited in the synthesis of a wide range of fullerene-based molecules.

This work establishes that C_{60} *has* a sonochemistry and points the way toward the sonochemical synthesis of novel fullerene derivatives. In particular, given that fullerenes are considered promising candidates for hydrogen storage, the discovery of a sonochemical route for the hydrogenation of fullerenes may be of importance for energy-storage applications. This work also establishes that fullerenes are an excellent probe of the sonochemical environment.

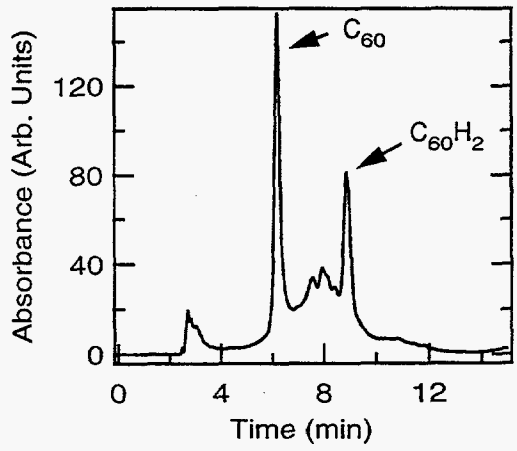

Fig. 1. Chromatogram of an ultrasonically irradiated sample of C_{60} in decahydrnaphthalene.

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1. Summary of paper: *J. Phys. Chem.* **101**, 123 (1997).
2. The University of Tennessee, Knoxville, Tenn.
3. Chemical and Analytical Sciences Division, ORNL.
4. ORNL/UT Distinguished Scientist.
5. K. S. Suslick, *Science* **247**, 1439 (1990).
6. L. A. Crum, *J. Acoust. Soc. Am.* **95**, 559 (1994).

THE FORMATION OF METAL/METAL-MATRIX NANOCOMPOSITES BY THE ULTRASONIC DISPERSION OF IMMISCIBLE LIQUID METALS[1]

V. Keppens,[2] D. Mandrus, J. Rankin,[3] and L. A Boatner

The special properties that can be obtained by forming metal-matrix composites have previously been extensively documented. While much of the prior attention has been focused on metal matrices reinforced with ceramic particles or fibers, the results reported for metal/metal-matrix materials show that the latter are no less interesting.

In the present work, a new approach to the formation of bulk metal/metal-matrix is presented. High-intensity ultrasound has been used to disperse one metallic liquid in a second immiscible liquid metal, thereby forming a metallic emulsion. When this emulsion is cooled, a metal/metal-matrix composite consisting of minor-phase particles dispersed in the solidified major phase is formed.

In order to investigate the application of ultrasound to the formation of metal/metal-matrix composites, the Zn-Bi case was selected as a model system. The composition selected for the present experiments consisted of 10 wt.% Bi. The composite metal/metal-matrix sample obtained after the sonication of the Zn-Bi melt has been characterized using scanning electron microscopy and energy-dispersive x-ray analysis. This analysis clearly shows that the Bi-phase forms essentially spherical particles that are embedded in the Zn-matrix. The dispersion is, however, far from homogeneous. Bi-particles with diameters ranging from more than 50 μm to less than 0.5 μm can be detected.

The presence of the submicron particles of Bi indicates that the application of high-intensity ultrasound can be a powerful tool for the formation of nanocomposite materials through the creation of metallic emulsions. However, the major problem to be overcome in future experiments is achieving an improvement in the monodispersed size-distribution of the minor-phase particles.

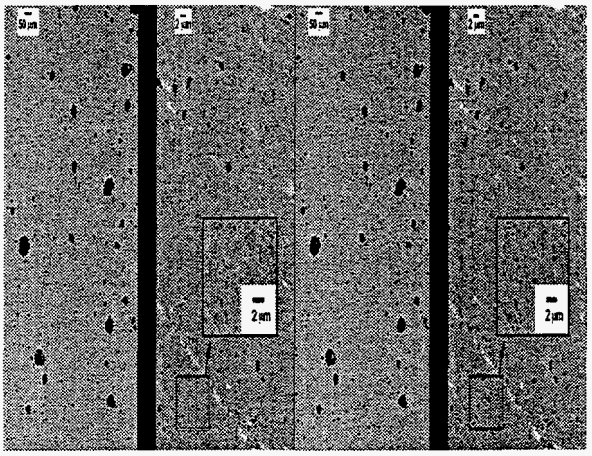

Fig. 1. (a) and (b) SEM image of a Zn-Bi composite obtained by conication of the two molten immiscible liquid metals.

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1. Summary of paper: *Mat. Res. Soc. Symp. Proc.* (in press).
2. ORNL/ORISE postdoctoral research associate.
3. Brown University, Providence R.I.

PREDICTING THE EFFECTS OF METAL CATIONS ON THE EASE OF GLASS FORMATION[1]

B. C. Sales, L. A. Boatner, and J. O. Ramey

The free energy of formation of a crystalline solid provides a measure of the thermodynamic driving force for the creation of a particular compound. It has been hypothesized since the early days of glass science that a small value for the free energy of formation implied that glasses made near this composition should exhibit a wider distribution of silicate anions and, hence, should form glasses more easily. This hypothesis is difficult to test in silicate, borate, and germanate glasses because of the inability to obtain reliable information about the distribution of anions in these glasses and the tendency of these glasses to phase separate. Precise information about the distribution of phosphate anions (chains of corner-linked PO_4 tetrahedra) in most metal-phosphate glasses, however, can be determined using high-performance liquid chromatography (HPLC). Phosphate glasses also show less of a tendency to phase separate and, thus, provide model systems to test some fundamental ideas about the role of various metal cations in glass formation.

The width of the phosphate anion distribution was measured for a variety of metal-phosphate glasses using the HPLC technique. The wider the distribution of phosphate anions, the greater the ease of glass formation. The ease of glass formation correlated well with literature values for the free energy of formation of the crystalline orthophosphates measured with respect to P_2O_5 and the metal oxide. The ease of glass formation did not correlate as well with the metal-oxygen field strength, a parameter frequently used in the glass industry. These results can be used to design glasses with better physical and chemical properties.

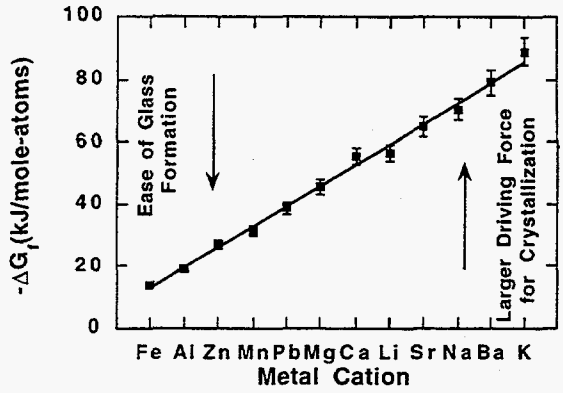

Fig. 1. Free energy of formation of the crystalline orthophosphates with respect to P_2O_5 and the metal oxide. A large energy of formation implies a strong driving force for crystallization and a narrow distribution of phosphate anions in the glass. A small energy of formation facilitates the formation of a glass with a wide distribution of phosphate anions.

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1. Summary of paper to be published.

ELECTRICAL PROPERTIES OF POLYETHYLENE HIGHLY FILLED WITH CARBON[1]

F. A. Modine, A. R. Duggal,[2] D. N. Robinson,[3] E. L. Churnetski,[3] M. Bartkowiak,[4] G. D. Mahan,[5] and L. M. Levinson[2]

Carbon-filled polyethylene composites exhibit a large positive temperature coefficient of resistance (PTCR). The resistance can change by orders of magnitude for a temperature change of a few degrees when the composites are heated through the polyethylene/crystalline melting transition. A series of such composites was fabricated and tested to establish the practical lower limit for the electrical resistivity at room temperature in materials with a PTCR effect large enough to be useful. The carbon type and content were systematically varied, and homogeneity was controlled by varying the number of passes through an extruder.

Carbon with a large particle size and low surface area provided low-resistivity composites with large PTCR anomalies. Figure 1 shows measurements made on a material having a room-temperature resistivity near the lower limit of that attained and a resistivity change of 2 orders of magnitude.

The PTCR anomaly was largest in composites that were well mixed and/or heated repetitively through the crystalline/melting transition. Figure 2 shows the increase in the PTCR anomaly as measured by the resistivity switching ratio ρ_{max}/ρ_{300} in a material repetitively cycled through the crystalline/melting transition.

It is doubtful that composites can be made with room-temperature resistivities that are much lower because the resistivities of carbon blacks are about 0.1 ohm-cm.

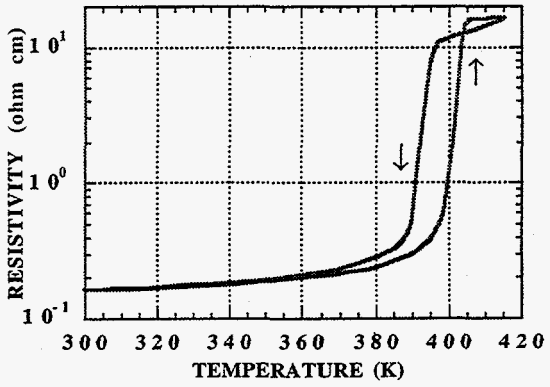

Fig. 1. Resistivity vs. temperature.

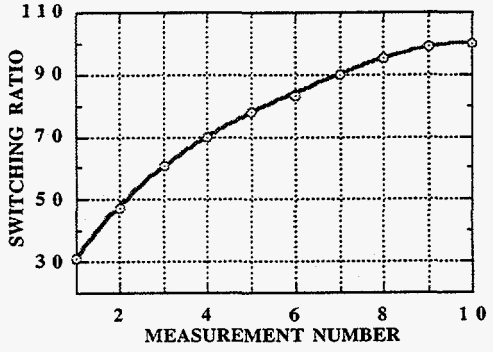

Fig. 2. Switching ratio vs. thermal cycling as gauged by measurement number.

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1. Summary of paper: *J. Mater. Res.* **11**, 2889 (1996).
2. General Electric Co., Schenectady, N.Y.
3. Development Division, Oak Ridge Y-12 Plant.
4. ORNL/ORISE postdoctoral research associate.
5. ORNL/UT Distinguished Scientist.

Chapter 4

Ion Beam and Laser Processing

Ion Beam Processing

FORMATION OF ORIENTED COMPOUND SEMICONDUCTOR NANOCRYSTALS IN SILICON BY ION BEAM SYNTHESIS[1]

C. W. White, J. D. Budai, J. G. Zhu,[2] S. P. Withrow, and R. A. Zuhr

The formation of nanocrystals and quantum dots has attracted considerable interest recently because the properties of these novel structures can differ considerably from those of bulk material because of quantum confinement effects. Ion implantation has been used to form a wide range of encapsulated nanocrystals and quantum dots in matrices such as Al_2O_3 and SiO_2. In these materials, ion implantation is used to inject an insoluble impurity into the near surface to form a supersaturated solution, and thermal annealing gives rise to precipitation and the formation of nanocrystals. Compound semiconductors are formed by implanting both constituents of the compound at energies chosen to give an overlap of the profile.

High-dose ion implantation has also been used to form compound semiconductor nanocrystals and quantum dots in the surface of silicon. Figure 1 shows x-ray diffraction Θ-2Θ scans along the [100] direction of silicon crystals implanted by various combinations of Group-III and Group-V ions. In each scan, the intense Si(004) reflection is observed; but in addition, there are strong peaks which arise from zincblende GaAs, GaP, InAs, and InP, showing that these compounds were formed as a result of implantation and annealing and that the nanocrystals are oriented with their (001) planes parallel to the Si(001) planes. These nanocrystals are also oriented in plane with their cube axes parallel to those of Si; thus, they are three dimensionally oriented with respect to the Si matrix. In addition to Group-III–V compound semiconductors, Group II–VI compound semiconductors have been produced in Si by implanting various combinations of Group-II and Group-VI ions. For these compound semiconductors, the structure produced is the cubic structure which is responsible because Si is a cubic material. The driving force for the formation of these compound semiconductor nanocrystals in silicon is their strong chemical affinity for each other, and the free energy of the desired compound relative to that of other possible compounds or the free energy of mixing of Si solid solutions provides a criterion to determine whether the compound will form, assuming there are no kinetic barriers.

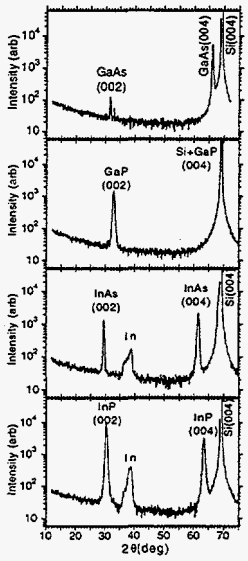

Fig. 1. X-ray diffraction results showing the formation of Group-III–V compound semiconductors as a result of sequential implantation. Equal doses of each ion were implanted at energies chosen to give an overlap of the profile. Implants were done at 500°C, and samples (a), (b), and (d) were subsequently annealed at 1000°C/1 h.

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1. Summary of papers: *Appl. Phys. Lett.* **68**, 2389 (1996); *Nuclear Instruments and Methods in Physics Research, Section B* (in press).

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SYNTHESIS, OPTICAL PROPERTIES, AND MICROSTRUCTURE OF SEMICONDUCTOR NANOCRYSTALS FORMED BY ION IMPLANTATION[1]

J. D. Budai, C. W. White, S. P. Withrow, R. A. Zuhr, and J. G. Zhu[2]

Motivated by the unique optoelectronic properties resulting from spatial confinement in quantum dots, a wide range of semiconducting nanocrystals encapsulated in the surface region of insulating substrates using high-dose ion implantation, followed by annealing, have been formed. Nanocrystalline precipitates have been successfully formed from groups IV (Si, Ge, SiGe), III–V (GaAs, InAs, GaP, InP, GaN), and II–VI (CdS, CdSe, CdS_xSe_{1-x}, CdTe, ZnS, ZnSe) in fused silica, Al_2O_3, and Si substrates.

Ion doses ranged up to ~10^{17}/cm^2 for each species, and the ion energies were chosen such that the ion concentration profiles were superimposed after implantation. As expected, the size of the nanocrystals increased when the substrate temperature was increased, either during implantation or during subsequent annealing. Structural characterization revealed that the nanocrystals embedded in amorphous SiO_2 possess nearly spherical shapes and random orientations, and nanocrystals formed in crystalline α-Al_2O_3 exhibit greater shape anisotropy, faceting, and specific crystallographic orientations.

Optical characterization revealed blue-shifts, in good agreement with theoretical estimates of size-dependent quantum-confinement energies of electrons and holes. Figure 1 shows the optical absorption coefficient measured after annealing at 1000°C for 1 h from 4 samples with different excess concentrations ranging from ~0.5 at. % to ~8 at. % for each of the implanted Cd and S ion species. As the concentration is decreased, the absorption threshold shifts toward shorter wavelength, as expected from quantum-size effects due to confinement of an electron and hole in nanocrystals smaller than the exciton Bohr diameter (~50 Å for CdS).

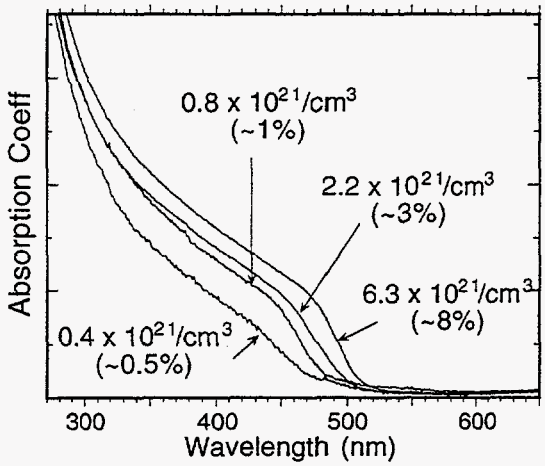

Fig. 1. Optical absorption coefficient for samples implanted with Cd and S ions to four different concentrations.

The shifts of the energy band gap extracted from these measurements are in good agreement with theoretical calculations of the quantum confinement energy, ΔE_g. This work demonstrates the potential of ion implantation as a synthesis technique for controlling the optoelectronic properties of nanostructured materials.

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1. Summary of paper: *Mat. Res. Soc. Symp. Proc.* 452, 89 (1997).

2. ORNL/ORISE postdoctoral research associate: Present address: New Mexico State University, Las Cruces, N. Mex.

OPTICAL PROPERTIES OF Si NANOCRYSTALS FORMED IN SiO_2 USING ION IMPLANTATION

S. P. Withrow, C. W. White, J. D. Budai, J. G. Zhu,[1] and D. M. Hembree, Jr.[2]

Nanocrystals have attracted significant attention recently because of their unusual properties, which result when structures are made significantly small that electrons are forced to be confined in regions smaller than their delocalized length. Si nanocrystals are of particular interest because they exhibit optical properties that have potential applications to optoelectronic devices. One technique for the formation of Si nanocrystals is ion implantation of Si into SiO_2 followed by thermal annealing; at sufficiently high temperatures, the implanted Si precipitates out from the SiO_2 matrix in the form of nanocrystals. The size of nanocrystals formed using this processing technique depends on the initial implantation concentration, the annealing temperature, and the annealing time.

Si nanocrystals, synthesized in SiO_2 by ion implantation followed by annealing above ~900°C in a forming gas ambient (Ar + 4%H_2), exhibit strong photoluminescence (PL) with the intensity peaked in the near-infrared region. A shift in the luminescence to higher energies is observed as the particle size decreases, which is expected from quantum confinement if the PL results from radiative recombination of bound excitons in the Si nanocrystals. However, the energy shift of the peak PL energy is very small over the dose range investigated. For samples in which most of the nanoparticles are larger than the delocalized length, the PL is weak.

The PL intensity (but not the peak wavelength) is very sensitive to the presence of hydrogen in the sample or annealing environment. The photoluminescence from samples initially annealed in Ar + 4%H_2 dramatically decreases following an anneal in vacuum. The PL can be restored fully by a subsequent reanneal in a forming gas ambient.

Si nanocrystals give rise to strong optical absorption. However, the dominant absorption edge is in the ultraviolet, while the photoluminescence is in the near infrared and exhibits a red shift of ~2.5 eV relative to the absorption edge. The fact that the absorption and PL occur at significantly different energies suggests that they may be related to different mechanisms. The PL arising from Si nanoparticles in SiO_2 cannot be attributed to the conventional band-edge luminescence.

These phenomena can be explained by a model in which the optical absorption is dominated by size-dependent quantum confinement in the nanoparticles. Absorption leads to electron hole pairs, but the excitation energy is transferred nonradiatively to interface states. The PL originates from transitions involving interface states, which are expected to have energies relatively independent of the particle size. Hydrogen is known to passivate the interface states, which can explain the sensitivity of the PL to the presence of H in the annealing ambient.

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ENHANCED DOPANT DIFFUSION IN VACANCY SUPERSATURATIONS PRODUCED BY MeV IMPLANTATION[1]

V. C. Venezia,[2] T. E. Haynes, A. Agarwal,[3] H.-J. Gossmann,[4] and D. J. Eaglesham[4]

Ion implantation in silicon produces distributions of interstitials and vacancies. For high-energy ion implantation, the spatial separation between these distributions is large enough that a net point-defect imbalance is created. The imbalance consists of interstitials and interstitial clusters near the ion's projected range and vacancies and vacancy clusters in the near-surface region. This work is aimed at isolating the vacancy-rich region from the interstitial-rich region to enable studies of defect-defect and dopant-defect interactions in large vacancy supersaturations.

The defect regions produced by a 2-MeV Si implant were isolated by implanting into a silicon-on-oxide (SOI) substrate. In this way, the interstitial-rich region was produced on the deep side of a SiO_2 barrier while the vacancy- rich region was produced on the shallow side. The diffusion of Sb dopant markers was used to monitor the injection of vacancies in the near-surface region. Experiments were also performed in float-zone (FZ) Si-(100) for comparison.

It was observed that the diffusion of Sb in the FZ substrate was enhanced by at least 20×, at 1000°C, as a result of the MeV implant. In the SOI substrate, the diffusion of Sb was enhanced by at least 40× for the same conditions, indicating a higher vacancy concentration in the SOI. This higher vacancy concentration is attributed to the oxide acting as a barrier to interstitials, preventing their diffusion to the vacancy-rich region and recombination. It was also observed that the enhancement in Sb diffusion decreased to 10× as the annealing time was increased from 20 to 60 min (i.e., the enhancement is transient). The fact the enhancement decreased with an increase in annealing time suggests that the vacancy concentration is decreasing with time.

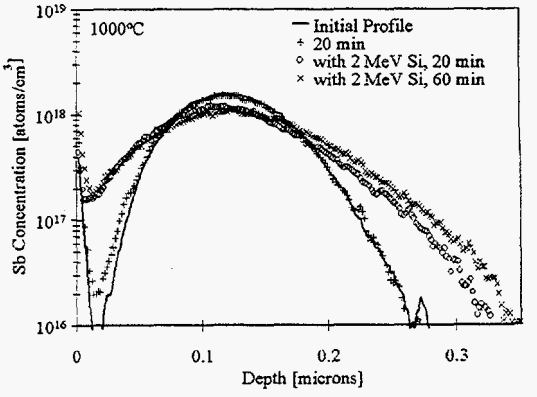

Fig. 1. Sb concentration profiles in SOI showing the initial Sb marker, annealed at 1000°C followed by 20-min anneal, implanted with MeV Si^+, and implanted with MeV Si^+ followed by a 60-min anneal.

As high-energy ion implantation becomes more widely used in silicon processing, understanding the behavior of defects and dopants in vacancy supersaturations will become essential. It has been demonstrated that the vacancy-rich region produced by MeV implantation can be isolated from interstitials deeper in the bulk. In this way, a "vacancy implanter" which can be used to answer fundamental questions on defect-defect and dopant-defect interactions in vacancy supersaturations has been created.

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1. Summary of paper to be published.
2. ORISE graduate laboratory participant from University of North Texas, Denton, Tex.
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SUPPRESSION OF TRANSIENT-ENHANCED DIFFUSION OF IMPLANTED BORON IN Si[1]

E. G. Roth[2] and O. W. Holland

A major problem in the manufacture of integrated circuits using ≤0.25-μm design rules is controlling the depth of electrical junctions formed by implantation. Despite the use of low-energy ions, junction depths remain anomalously deep. This has been shown to be the result of ion-induced defects which produce a transient-enhanced diffusion of the dopant during annealing. The transiency can increase the dopant diffusivity by orders of magnitude and persists until the defects are either eliminated from the diffusion volume or become trapped. In particular, the diffusivity of the implanted boron is enhanced by a factor of ≥1000 because of excess interstitials.

A method of controlling transient-enhanced diffusion of boron was devised which involved implantation of high-energy, Si^+ self-ions. High-energy ions create a vacancy-rich region near the surface. A silicon-on-insulator material (consisting of a ~1-μm layer of Si bonded to a thermally grown SiO_2 layer on bulk Si) was chosen for this experiment to ensure that only vacancies were injected into the top Si layer during the self-ion irradiation. Therefore, self-ions and boron were co-implanted at energies which overlap the interstitials from the boron implant with the vacancy-rich region formed by the self-ions to create a situation where the defects can mutually annihilate. The co-implantation was done using 40-keV B^+-ions at a dose of 10^{14} cm^{-2} and 2-MeV Si^+-ions at a dose of 5×10^{15} cm^{-2}. Figure 1 compares the boron profiles for various conditions. It is clear that the diffused profiles (after 800°C annealing) demonstrate that the motion of the boron within the co-implanted sample has been substantially retarded over the control (i.e., a B^+-only implanted sample). This technique of engineering defect profiles appears to be quite effective in limiting the diffusion of boron and, thus, the depth of electrical junctions.

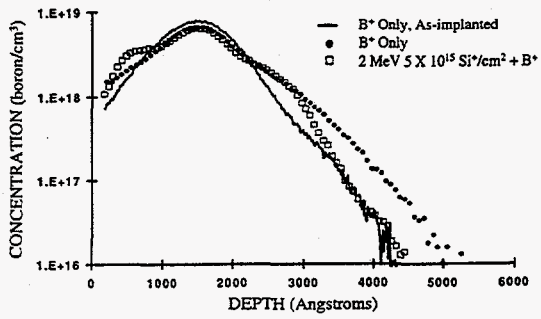

Fig. 1. Comparison of boron profiles obtained by secondary ion mass spectroscopy. The profile after annealing at 800°C/15 min. in the sample implanted only with B^+ ions demonstrates the effects of transient-enhanced diffusion. The profile is seen to penetrate ~1000 Å beyond the as-implanted one. The co-implanted profile exhibits much less diffusion.

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1. Summary of paper: *Journal of Electronic Materials* (in press).

2. ORISE graduate laboratory participant from the University of North Texas, Denton, Tex.

INTERSTITIAL DEFECTS AND TRANSIENT-ENHANCED DIFFUSION FROM VERY LOW ENERGY IMPLANTATION IN SILICON[1,2]

A. Agarwal,[3] T. E. Haynes, D. J. Eaglesham,[4] H.-J. Gossmann,[4] L. Pelaz,[4] D. C. Jacobson,[3] and J. M. Poate[4]

Ion implantation injects large numbers of point defects (interstitials and vacancies) into the crystal. In silicon, the interstitials greatly enhance the diffusion of dopants, such as B, during postimplant annealing. Future silicon technology will require implant energies below 1 keV for doping so that both defects and dopants will be injected at larger concentrations and closer to the surface. This research is aimed at understanding changes in defect and dopant behavior caused by increased interaction with the surface and with each other.

The evolution of defects and diffusion following ion implantation in silicon at energies between 0.5 and 5 keV has been examined experimentally. It has been observed that interstitial concentrations larger than ~1% produce corrugated "zigzag" defects by the intersection of simpler {311}-type defects (Fig. 1) during annealing at 700°–900°C. These defects act as sources of free interstitials at longer times, and their stability extends the time of the enhanced diffusion. The diffusion of interstitials into the bulk, monitored by B-doped markers, was found to decrease as the interstitial source was moved closer to the surface indicating that the surface is a nearly perfect sink for the interstitials after they are emitted from zigzag defects. For concentrations of implanted B in excess of ~5%, an amorphous phase is formed that remains stable during annealing up to at least 1050°C for several hours. From electron diffraction, this phase has tentatively been identified as a-SiB_4.

Transient-enhanced diffusion (TED) will soon become the chief factor limiting the use of ion implantation for shallow silicon doping. Processing parameters that will be required in 10 years have been investigated, and it has been shown that when the implant energy is reduced, TED will decrease sufficiently to enable the continued use of ion implantation in silicon technology.

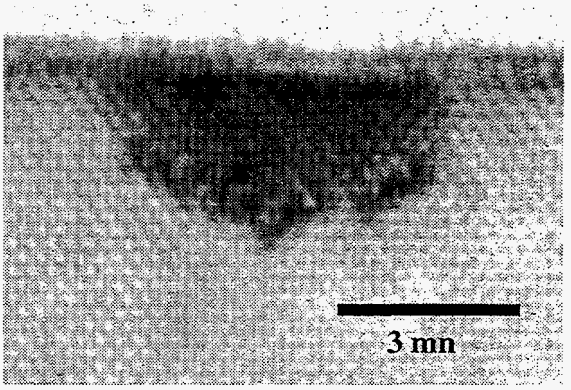

Fig. 1. High-resolution cross-section micrograph in {110} projection showing a zigzag defect consisting of four {311}-type segments located less than 2 nm from the surface of a silicon sample following implantation and annealing.

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1. Summary of papers: *Applied Physics Letters* (in press); to be published.

2. Partially supported through a CRADA with Lucent Technologies sponsored by the Laboratory Technology Research Program, Office of Energy Research.

3. ORNL/ORISE postdoctoral research associate.

4. Bell Laboratories, Lucent Technologies, Murray Hill, N.J.

TECHNIQUE TO FORM ULTRATHIN BURIED OXIDES IN Si BY O^+ IMPLANTATION[1]

O. W. Holland

Silicon-on-insulator (SOI) material is projected for use as the starting substrate of future generations of integrated circuits. This composite material consists of a buried-oxide (BOX) layer which isolates the top Si layer from the bulk. O^+ implantation of Si is used to fabricate SOI but is costly and suffers from residual defects in the top layer of Si. Both these issues relate to the magnitude of the implantation dose which can be substantially overcome by simply utilizing a smaller dose (i.e., 3×10^{17} cm^{-2} rather than a typical dose of ~2×10^{18} cm^{-2}). However, success of this approach is problematic since simply reducing the implant dose results in the formation of a discontinuous oxide layer which fails to electrically isolate the top Si layer. A two-step implantation scheme was developed to overcome this problem. The first step consists of a standard implant to introduce sufficient oxygen into the lattice to yield a target thickness for BOX. It is done at high temperature, ≥500°C, to maintain the crystallinity of the lattice. The second step utilizes the same O^+ beam but is applied near room temperature (RT) to selectively amorphize the region where the BOX forms (during postimplantation annealing). The amorphous layer promotes formation of a continuous BOX during subsequent furnace annealing. Crystallization of the amorphous layer during annealing results in polycrystalline rather than single-crystal growth because of the high concentration of implanted oxygen. The grain boundaries of the polycrystal promote rapid diffusion of the implanted oxygen, thus enhancing the susceptibility of the oxide to form continuously. Cross-section, transmission electron micrographs (XTEM) demonstrate the efficacy of this two-step technique. It is clear that in Fig. 1(a), a single-step process results only in isolated oxide precipitates while in Fig. 1(b), application of the two-step technique yields a completely continuous BOX.

1. Summary of paper: *Appl. Phys. Lett.* **69**, 674 (1996).

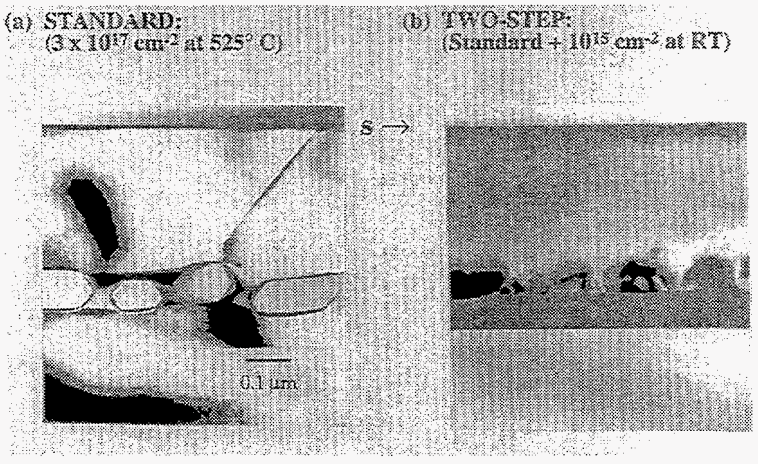

Fig. 1. XTEM from 1300°C annealed Si implanted using (a) the standard process consisting of implantation at 525°C of 150 keV O^+ ions at a dose of 3×10^{17} cm^{-2} and (b) a two-step method consisting of the standard process followed by a 10^{15} cm^{-2} dose at RT.

ION BEAM MODIFICATION OF INDIUM-TIN-OXIDE FILMS[1]

T. E. Haynes, Y. Shigesato,[2] I. Yasui,[2] N. Taga,[3] and H. Odaka[3]

Indium-tin-oxide (ITO) is the transparent conductor having the best known combination of optical transmission and conductivity, so that ITO films are an important enabling material for a growing range of applications, including displays, photovoltaics, and smart materials. ITO is a wide band-gap semiconductor with carrier electrons donated by tetravalent-Sn donors and oxygen vacancies. Conductivity changes induced in optimized ITO films have been investigated by ion implanting various species in order to separate the contributions from chemical doping and crystal defects to the resistance and to evaluate prospects for postdeposition film engineering for applications.

Polycrystalline ITO films ($\rho_0 = 190\ \mu\Omega$-cm, and $n_0 = 9 \times 10^{20}\ e^-/cm^3$) were implanted with H^+, O^+, In^+, N^+, F^+, Ne^+, and Ar^+ ions. At concentrations up to ~$5 \times 10^{20}/cm^3$, all ions slightly degrade the conductivity, an effect dominated by deactivation of Sn donors. However, when the implant concentration exceeds $1 \times 10^{21}/cm^3$, chemical effects that depend upon the ion species are observed.(Fig. 1). With some ions (e.g., In^+), it is possible to obtain small reductions in resistivity, but others lead to large increases. The latter effect is associated with compensation of the O-vacancy donors. Figure 1 shows that O^+ ions are much more effective in this process than either of the neighboring elements in the periodic table (N^+ or F^+), which in turn are more effective than the inert gases (e.g., Ar^+).

Single-crystal films enable more thorough defect characterization for basic studies. Ion implantation into single-crystal ITO films grown by molecular beam epitaxy has been investigated. Ion channeling detected saturation of damage growth vs. dose corresponding to the saturation

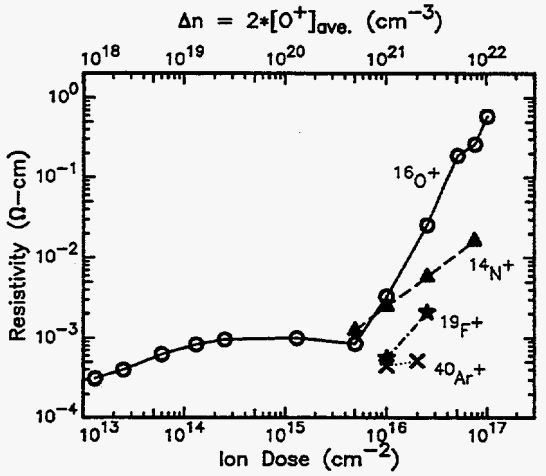

Fig. 1. Conductivity changes induced in ITO films by implantation of N^+, O^+, F^+, and Ar^+.

of resistivity at doses near $10^{14}/cm^2$. Earlier, it had been proposed that such damage saturation was based on studies of polycrystalline films but the damage could not be measured. These new results indicate that the saturation of damage and resistivity is intrinsic to the crystal chemistry (i.e., it is not associated with grain boundaries).

Properties of ITO films are dominated by defects incorporated during growth. Ion implantation provides a tool to controllably inject point defects and dopants separately into thin films and to do so independently of growth conditions. These studies have led to an improved understanding of the fundamental mechanisms controlling the properties of these films. These results demonstrate the ability to control film properties after deposition, which permits more flexibility for patterning and processing of these important transparent conducting films.

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1. Summary of paper: *Nucl. Instrum. Methods Phys. Res. B* **121**, 221 (1997).
2. University of Tokyo, Tokyo, Japan.
3. Asahi Glass Co., Yokohama, Japan.

BORON SUBOXIDE SYNTHESIS USING ELECTRON CYCLOTRON RESONANCE MICROWAVE PLASMAS

S. M. Gorbatkin,[1] C. Doughty,[2] D. B. Poker, and R. L. Rhoades[3]

There is a continuing need for thin material layers with improved resistance to friction and wear for applications such as power generation, machining, and optics. Boron suboxides (B/O atom ratios > 1) are an attractive class of hard materials which, similar to diamond and cubic-BN, have been synthesized in bulk forms for over 25 years using high temperatures and pressures. Recently, boron suboxide phases capable of scratching diamond have been synthesized.[4] Also, lubricating films have been formed from B_2O_3.[5] Thus, it may be possible to form a lubricating surface on top of a hard thin film using only boron and oxygen. Despite these encouraging results, little attention has been devoted to depositing boron suboxides in thin-film form.

In this research, magnetron sputtering was used to inject elemental boron into an Ar electron cyclotron resonance microwave plasma for thin-film deposition. Boron suboxide films with B/O ratios varying from 0 to 1 were synthesized, and the resulting hardnesses were measured and found to vary from 2 to 40 GPa, with the lowest oxygen content producing the hardest films (Fig. 1). Films as deposited are amorphous and exhibit excellent adhesion to Si substrates and resistance to common acids and solvents, in marked contrast with elemental B films.

Further work will investigate annealing and wear behavior under varying atmospheric conditions.

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1. Present address: Emory University, Atlanta, Ga.
2. ORNL/ORISE postdoctoral research associate. Present address: PlasmaQuest, Inc., Richardson, Tex.
3. ORNL/ORISE postdoctoral research associate. Present address: Solution Technology, Monroe, N.C.
4. A. R. Badzian, *Appl. Phys. Lett.* 53, 2495 (1988).
5. A. Erdemir, *Res. Dev.* 33(11), 75 (1991).

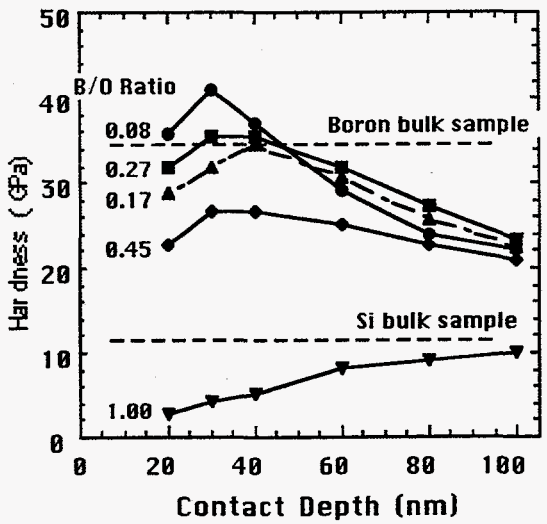

Fig. 1. Nanoindentation hardness vs. contact depth for boron suboxide films of varying B/O ratio, as indicated to the left of each curve.

SURFACE HARDNESS ENHANCEMENT OF ION-IMPLANTED AMORPHOUS CARBON[1]

D.-K. Lee,[2] H. Lee,[2] B. Park,[2] D. B. Poker, and L. Riester[3]

There have been numerous attempts to produce the expected superhard phase of carbon nitride, with no confirmed success. Efforts to produce the phase by nitrogen implantation of amorphous carbon, however, have produced significant increases in the surface hardness and elastic modulus of the material. Implantation of 100-keV nitrogen ions to a dose of 2×10^{17} cm^{-2} produces a threefold increase in the surface hardness (Fig. 1). The effect, however, has a strong temperature dependence, requiring sample temperatures below about 300 K during implantation to produce the full effect.

Raman spectroscopy was employed to characterize changes in vibrational modes for various N^+ implantation temperatures. The enhanced hardness and modulus at low temperatures are well correlated with an asymmetric diffuse peak around 1500 cm^{-1} and a broad band at ~700 cm^{-1}. The asymmetric peak has been associated previously with diamondlike carbon,[4] while the broad band has been observed in inert gas-implanted C, and was attributed to disorder in the material.[5]

From the results of this study, it is not possible to determine whether the enhanced hardness and modulus are the result of the formation of carbon nitride bonds or from the formation of diamondlike carbon. Further studies are expected to identify the relaxation mechanisms of the structural defects associated with the enhanced hardness and modulus effects, as well as the effects on the Raman vibrational modes.

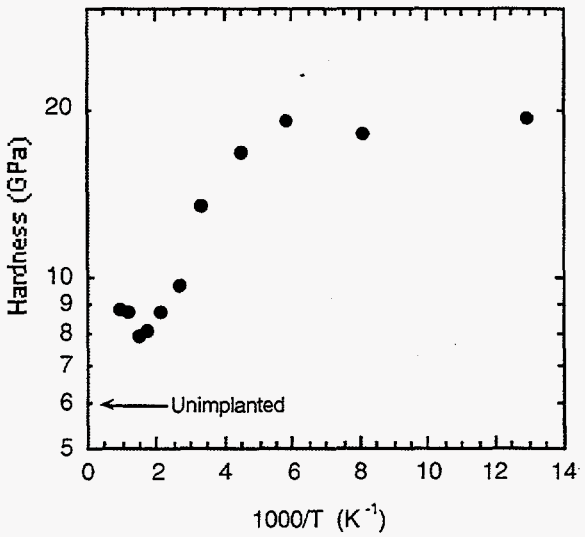

Fig. 1. Hardness vs. inverse temperature of amorphous carbon implanted with 100-keV nitrogen to a dose of 2×10^{17} cm^{-2}.

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1. Summary of paper: *Appl. Phys. Lett.* **70**, 3104 (1997).
2. Georgia Institute of Technology, Atlanta, Ga.
3. Metals and Ceramics Division, ORNL.
4. D. S. Knight and W. B. White, *J. Mater. Res.* **4**, 385 (1989).
5. F. Parmigiani, E. Kay, and H. Seki, *J. Appl. Phys.* **64**, 3031 (1988).

IRRADIATION EFFECTS IN MgF_2 COATINGS ON Si AND GaAs SUBSTRATES[1]

G. C. Farlow[2] and L. A. Boatner

The reduction of the reflection of light from a surface through the application of a coating with an appropriate thickness and index of refraction is a widely used technique. Because a high degree of adhesion between an anti-reflection coating and the underlying substrate is necessary in practical optical components, new approaches for improving the properties of coating-substrate interfaces are desirable. Previous studies have shown that ion irradiation is useful in enhancing the adhesion between films and substrates. Heavy-particle radiation effects and potential associated ion beam mixing effects were investigated for the purpose of promoting bonding between MgF_2 coatings and the semiconducting substrates Si and GaAs—materials that are important for photovoltaic and electro-optic devices whose efficiency is affected by the amount of light transmitted into the electronically active regions of the material.

The nature of the ion-beam-induced alterations of ~53-nm-thick films of MgF_2 deposited on Si or GaAs substrates and subsequently irradiated with 210-keV $^{132}Xe^+$ ions was studied using Rutherford backscattering (RBS) and scanning electron microscopy (SEM). Each sample consisted of a MgF_2-coated single crystal having four separate regions. One region was masked and unirradiated, and the remaining three regions were irradiated with ^{132}Xe.

Figure 1 shows an SEM micrograph for an MgF_2 film on a GaAs substrate for an area where the regions receiving different doses of Xe ions intersect. Region **a** in the lower left-hand corner of the SEM micrograph received no radiation; region **b** received 0.5×10^{16} Xe ions/ cm^2; region **c**: 1×10^{16} Xe ions/cm^2; and region **d**: 1.5×10^{16} Xe ions/cm^2. The film in area **a** is smooth and featureless, but the ion-irradiated regions in areas **b**, **c**, and **d** are eroded. These effects indicate that, as opposed to the case of MgF_2 optical coatings on LiF,[3] heavy-ion irradiation is not useful for improving adhesion between MgF_2 and either Si or GaAs.

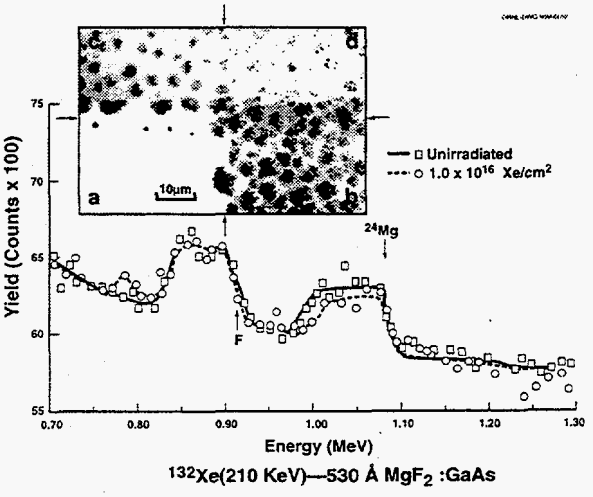

Fig. 1. RBS data from a 53-nm-thick MgF_2 film on GaAs in the unirradiated state and after irradiation with 1×10^{16} Xe ions/cm^2 at 210 keV. The inset is an SEM micrograph of the intersection of regions of the film that experienced different radiation doses: (a) unirradiated, (b) 0.5×10^{16} Xe ions/cm^2, (c) 1×10^{16} Xe ions/cm^2, (d) 1.5×10^{16} Xe ions/cm^2. The dark features in the portions that were irradiated are primarily pits eroded by the Xe-ion beam.

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1. Summary of paper: *Optical Materials* (in press).
2. Wright State University, Dayton, Ohio.
3. G. C. Farlow and L. A. Boatner, *Nucl. Instrum. Methods Phys. Res. B* **46**, 422 (1990).

ION EXCHANGE IN POTASSIUM TITANYL PHOSPHATE (KTP)[1]

K. Daneshvar,[2] E. A. Giess,[2] A. M. Bacon,[3] D. G. Dawes,[3] L. A. Gea,[4] and L. A. Boatner

Potassium titanyl phosphate, or KTP, is characterized by relatively large nonlinear optical and electro-optic properties, and accordingly, KTP has found applications in a variety of optical applications. Recently, attention has been focused on the formation of optical nonlinear waveguides on KTP substrates because of potential applications for compact and efficient generation of coherent light over a large wavelength range. Waveguides may be formed on KTP by thermal in-diffusion, ion exchange, or ion implantation. For waveguide formation by diffusion exchange, the diffusion depth determines the effective optical waveguide cross-section, which is an important parameter in the modal distribution, light propagation, and the induced electro-optic effect. It is essential that ion exchange parameters and mechanisms are determined for optimum waveguide construction.

Waveguiding regions can be formed in KTP by the ion exchange of K with Rb, Cs, or NH_4— either individually or combined. The process consists of immersing the KTP substrate in a molten solution $M(NO_3)_n$, where M is the ion that will exchange with potassium. Here, Rb replaced K, and the ion exchange processes in KTP immersed in Rb, Rb-Ba, and Rb-Sr nitrate molten solutions were investigated by using Rutherford backscattering (RBS) depth-profile analysis.

Using pure $RbNO_3$, the depth of the exchange was relatively shallow. However, the depth to which Rb-ion exchange occurred in KTP was found to be sensitive to the presence of as little as 0.1% of a Ba impurity in a molten solution of rubidium nitrate. The addition of impurities such as Ba significantly increased the ion exchange depth of Rb in KTP.

Figure 1 shows the RBS results for KTP samples ion exchanged for 1 h in molten rubidium nitrate with 0.1% and 1.0% Ba, respectively. These results show that Ba has a pronounced effect on the depth of penetration of Rb into the KTP surface, and the Rb diffusion depth in KTP increases progressively with the percentage of Ba in the melt. These findings are relevant to the application of ion exchange techniques to the fabrication of optical waveguides on KTP substrates.

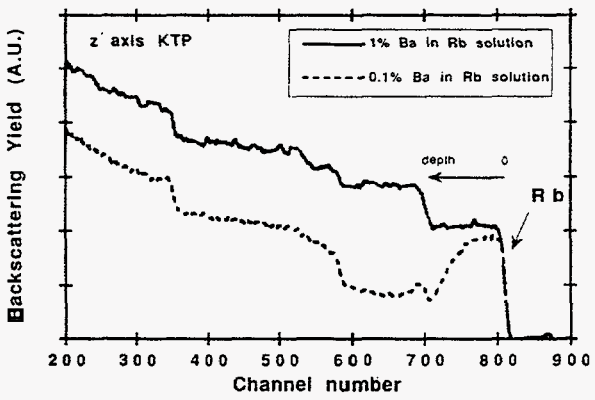

Fig. 1. RBS results for the negative z-axis surface of a KTP crystal ion exchanged in a $RbNO_3$ melt using a 0.1% and 1.0% $Ba(NO_3)_2$ impurity addition.

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1. Summary of paper: *Applied Physics Letters* (in press).
2. University of North Carolina at Charlotte, Charlotte, N.C.
3. Litton Airtron–SYNOPTICS, Charlotte, N.C.
4. ORNL/ORISE postdoctoral research associate.

STABILITY OF ION-IMPLANTED LAYERS ON MgO UNDER ULTRASONIC CAVITATION[1]

L. J. Romana,[2] J. Rankin,[3] J. R. Brewster,[4] L. A. Boatner, and A. M. Williams[5]

The effects of ion implantation on defect formation in MgO have previously been studied in detail. The implanted ions and associated defects can produce a volume expansion, and because the material is free to expand only normal to the surface, the stresses produced are usually compressive and biaxial in the surface plane. The combined effects of the large, static biaxial stresses introduced by ion implantation and the shock-wave forces resulting from ultrasonic-cavitation interactions on MgO single-crystal surfaces were investigated. The ultrasonic cavitation interactions arise from the impulsive force due to the rapid collapse of cavitation bubbles.

When the strained surface layers are subjected to an ultrasonic (~20-kHz) cavitation treatment, uniform layers (~100–200 nm) can be removed from the MgO surface in a controlled manner. The thickness of the removed layers is directly related to the duration of the ultrasonic irradiation but does not exceed the depth of the implanted species. The removal process appears to be independent of the MgO crystallographic orientation and of the chemical nature of the implanted ions.

When MgO implanted with Ar^+ or Kr^+ at fluences of 5×10^{16}–10^{17} ions cm^{-2} is irradiated with 2-MeV He^+ ions at 10^{16}–10^{17} ions cm^{-2}, the region exposed to the He^+ beam is stabilized and is not removed by the ultrasonic treatment. For MgO implanted with $>2 \times 10^{17}$ K^+ ions cm^{-2}, the implanted layer is highly strained and detaches form the underlying crystal without exposure to ultrasonic cavitation, as shown in Fig. 1. These findings have applications in the mechanical "etching" of ceramics.

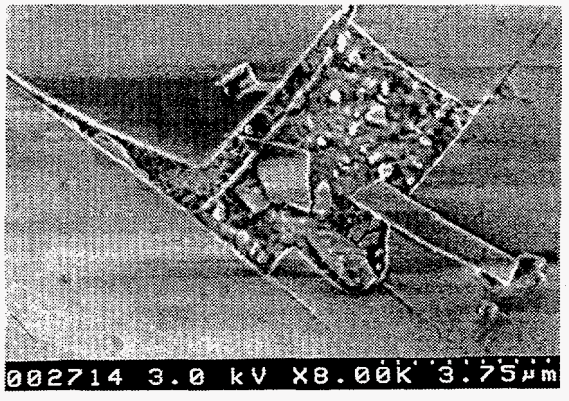

Fig. 1. Scanning electron micrograph of a (100)-oriented MgO single-crystal surface implanted with 2×10^{16} K^+ ions cm^{-2}. The spontaneous spalling of the surface is apparent as are the cleavage cracks along <100> directions. An adjacent portion of the thin surface layer is still intact but has peeled away from the underlying bulk material and is actually bent in response to the in-plane biaxial stress.

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1. Summary of paper: *J. Appl. Phys.* **80**, 2781 (1996).
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Laser and Molecular Beam Processing of Thin Films

PULSED-LASER ABLATION GROWTH AND DOPING OF EPITAXIAL COMPOUND SEMICONDUCTOR FILMS[1]

D. H. Lowndes and C. M. Rouleau[2]

Compound semiconductor (CS) electrical properties are far more sensitive to low defect concentrations than are the oxide ceramics for which pulsed-laser deposition (PLD) has been so successful. Only recently have doped epitaxial CS films been grown by PLD or fundamental studies carried out to relate their microstructural and electrical properties to the energy distribution of ablated species. Recently, these issues were reviewed using data obtained in this and other laboratories.

Rutherford backscattering measurements, though limited by ~1% precision, demonstrate that stoichiometric epitaxial CS films can be grown by PLD from a target of the same composition. However, congruent transfer does appear to be sensitive to ambient gas pressure and to the laser energy density focused on the target.

Highly doped *p*-type ZnTe:N films (~10^{20} holes/cm^3) have been grown by ablating a ZnTe target through molecular N_2. The high nitrogen doping is believed to be due to direct kinetic-energy induced reactions of Zn with N_2, probably on the growing film surface. Cluster/nanoparticle deposition occurs with increasing gas pressure. Nevertheless, experiments have demonstrated the feasibility of controlling film composition from the gas phase (e.g., $ZnSe_{1-x}S_x$ films were grown by ablation of a pure ZnSe target into ambient H_2S gas whose pressure was varied continuously to control the sulfur fraction, "*x*").

Doped, fully epitaxial films of $CuInSe_2$ (CIS) and of group-III nitrides also have been grown recently by PLD. Growth of epitaxial *n*-CIS at 350°C is promising because this is ~175°C below the temperatures at which polycrystalline CIS films are grown for solar cells, suggesting that it may be possible to grow various I-III-VI_2 family members at low temperatures and study their doping mechanisms. Similarly, GaN and InN films have been grown on sapphire (0001) substrates at ~500°C without the use of a buffer layer; this temperature is significantly lower than for most group-III nitride growth by molecular beam epitaxy or metal-organic chemical vapor deposition..

These examples emphasize the importance of the energetic ablation growth environment and the continuing need for in situ diagnostic measurements in order to develop a fundamental understanding of nonequilibrium CS growth and doping during PLD.

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1. Summary of papers: in *Laser Desorption and Ablation*, Academic Press, New York, 1997 (in press); *Mat. Res. Soc. Symp. Proc.* **397**, 107 (1996).
2. Eugene P. Wigner Fellow.

EFFECT OF AMBIENT GAS PRESSURE ON PULSED-LASER ABLATION PLUME DYNAMICS AND ZnTe FILM GROWTH[1]

C. M. Rouleau,[2] D. H. Lowndes, M. A. Strauss,[3] S. Cao,[3] A. J. Pedraza,[4] D. B. Geohegan, A. A. Puretzky,[5] and L. F. Allard[6]

Recently, the growth of thin epitaxial films of highly doped *p*-type ZnTe:N on GaAs(001) by pulsed-laser ablation (PLA) of a pure ZnTe target into varying pressures of ambient N_2 gas was reported. However, the hole mobility in these films was sharply peaked at a N_2 pressure of 50 mTorr, where the hole carrier concentration also exhibited a broader maximum. A combination of reflection high-energy electron diffraction (RHEED), cross-sectional transmission electron microscopy (XTEM), and in situ ion probe measurements have been used to discover why there is an optimum pressure for compound semiconductor growth and doping by PLA.

RHEED revealed a strong correlation between the film-growth mode and ambient N_2 pressure, with 2D growth for pressures <30 mTorr and 3D growth for higher pressures. The extended defect content (assessed via XTEM) in the region >150 nm from the film/substrate interface also was found to increase with N_2 pressure, which could not be explained by lattice mismatch alone. At N_2 pressures ≥ 100 mTorr, misoriented, columnar grains developed, consistent with both the RHEED observations (diffuse, spotty, low-contrast pattern) and the marked decrease in Hall mobility.

Ion probe measurements, which monitor the attenuation and slowing of the ion current arriving at the substrate surface, indicated that for increasing N_2 pressure the fast (vacuum) ion-velocity distribution splits into a distinct fast component and two collisionally slowed components. Three distinct pressure regimes in which each component in turn dominated the flux impinging on the substrate were formed. Component 1, dominant below ~15 mTorr and consisting of fast atoms and ions, produced films with the least number of extended defects, although point defects apparently still limit film optoelectronic properties in this regime. Component 2, dominant from ~15 to ~70 mTorr and consisting of collisionally slowed atoms and ions, seems to be necessary for high-quality doped films, as evidenced by a high carrier concentration and hole mobility. Lastly, component 3, which dominated the ion flux for pressures above ~70 mTorr, is consistent with the onset of cluster deposition. High-resolution XTEM later confirmed the presence of ~10-nm spherical clusters on and near the surfaces of films grown in this regime.

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1. Summary of paper: *Mat. Res. Soc. Symp. Proc.* **397**, 119 (1996).
2. Eugene P. Wigner Fellow.
3. Graduate student from The University of Tennessee, Knoxville, Tenn.
4. The University of Tennessee, Knoxville, Tenn.
5. ORNL/ORISE postdoctoral research associate.
6. Metals and Ceramics Division, ORNL.

NOVEL THIN-FILM MATERIALS SYNTHESIZED BY CONTROLLING THE PULSED-LASER DEPOSITION FLUX[1]

D. H. Lowndes, D. B. Geohegan, A. A. Puretzky,[2] D. P. Norton, and C. M. Rouleau[3]

Researchers in several laboratories recently found that by varying the laser wavelength and intensity and the ambient gas pressure, the nature of the pulsed-laser deposition (PLD) flux and its energy distribution can be controlled. Species ranging from energetic atoms and ions through clusters and nanoparticles can be produced, creating new opportunities to synthesize novel thin-film materials and control thin-film properties.

Films of hard, hydrogen-free amorphous diamond (a-D) with high sp^3:sp^2 bonding ratios can be produced by ArF (193-nm) pulsed-laser ablation of a graphite target at only moderate power densities (~10^8 W-cm^{-2}). In contrast, ablation using doubled Nd:YAG radiation (532 nm) requires power densities >10^{10} W-cm^{-2}. The reason for this strong laser wavelength dependence was understood only recently when temporally and spatially resolved images obtained at ORNL revealed three distinct components in the ablation plume. Carbon dimers (C_2), trimers (C_3), and clusters (C_n) with low kinetic energy (~0.2–1.7 eV) were found at low laser intensity. For higher intensity, C^+ ions with kinetic energies ~85 eV were formed. At equal intensity (~6.7 J/cm^2), the short-wavelength ArF (193-nm) laser plume was dominated by luminescence from the C^+ ions, whereas the KrF (248-nm) plume exhibited only weak C^+ luminescence. Thus, the dominance of fast ions and corresponding minimization of slower moving clusters appears to be the fundamental factor controlling the sp^3:sp^2 ratio in a-D films.

Cluster formation can be greatly enhanced by ablating a material into a moderate-pressure (0.1–10-Torr) ambient gas. By increasing the gas pressure, one can change the flux available for film deposition from primarily energetic atoms and ions to clusters. At pressures ≥1 Torr, nanocrystals are formed, typically with diams of 1 to 10 nm and containing from 10^2 to 10^5 atoms.[4]

Cluster-assembled or highly nanocrystalline films may have properties much different than films grown from predominantly atomic/ionic species, either because of quantum confinement effects or because entirely new, composite materials are formed. For example, luminescence and electroluminescence have been observed from nanocrystalline Si films produced by PLD into He gas, and composite organic:inorganic materials with high nonlinear optical activity also have been created at State University of New York–Buffalo by ablating a silica (SiO_2) rod into a He gas pulse in which an organic vapor was entrained.

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1. Summary of paper: *Science* 273, 898 (1996).
2. ORNL/ORISE postdoctoral research associate.
3. Eugene P. Wigner Fellow.
4. C. M. Rouleau et al., "Effect of Ambient Gas Pressure on Pulsed-Laser Ablation Plume Dynamics and ZnTe Film Growth," this Progress Report.

GAS-PHASE DIAGNOSTICS OF NANOPARTICLE SYNTHESIS BY LASER ABLATION INTO A BACKGROUND GAS[1]

D. B. Geohegan, A. A. Puretzky,[2] G. Duscher,[3] and S. J. Pennycook

Novel thin films containing nanoparticles can be grown by laser ablation into a background gas. Silicon ablation into helium or argon, for example, produces nanoparticles of silicon or silicon-rich silicon oxide (SRSO) in sizes where quantum confinement effects can alter photoluminescence properties. However, the dynamics and growth process of nanoparticle formation by laser ablation are virtually unknown.

Fundamental measurements of laser ablation plume dynamics resulting in gas-phase nanoparticle synthesis were made under various background gas and processing conditions. For the first time, intensified-CCD array photography and time-resolved optical emission spectroscopy were used to characterize the synthesis, transport, and deposition dynamics of luminescent SRSO nanoparticles formed and suspended in the gas phase. Secondary laser irradiation of the nanoparticles produced by KrF-laser ablation of silicon into 1–10-Torr argon or helium resulted in visible luminescence that peaked in argon from 390–470 nm with lifetimes of ~1–3 μs.

In situ imaging permitted direct monitoring of the formation and deposition processes (Fig. 1) as well as optimization of the flow conditions for photoluminescent nanoparticle formation.

Suspended 1–5-nm nanoparticles were swept onto TEM grids directly from the gas phase and imaged by Z-contrast STEM and compositionally profiled using EELS.

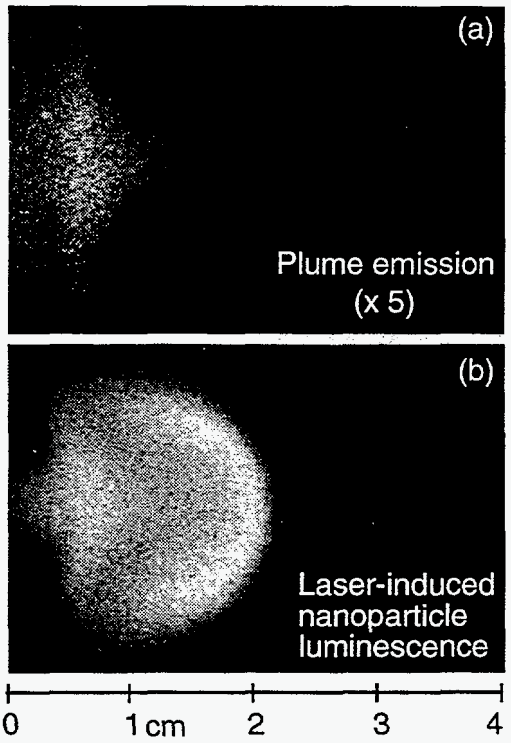

Fig. 1. Intensified CCD-array photographs (3-μs exposures) taken 400 μs after KrF-laser ablation of a silicon wafer into 10-Torr helium gas showing (a) remaining visible plume emission near the silicon wafer surface and (b) nanoparticle luminescence induced by passing a sheet of 308-nm light through the plume.

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1. Summary of paper to be published.
2. ORNL/ORISE postdoctoral research associate.
3. ORNL/ORISE/University of Illinois at Chicago postdoctoral research associate.

LASER-INDUCED FLUORESCENCE IMAGING AND GAS-PHASE DIAGNOSTICS OF LASER-DESORBED MALDI-MATRIX PLUMES[1]

A. A. Puretzky[2] and D. B. Geohegan

Laser desorption of organic crystals is now used routinely for mass-spectral analysis of large biomolecules, such as DNA fragments, which are intentionally encapsulated in the crystal matrix. In the matrix-assisted laser desorption ionization (MALDI) technique, the organic crystal absorbs the laser energy, the analyte biomolecule is ejected intact along with the plume of matrix material, and a fraction of the analyte molecules are ionized and detected by high-resolution mass spectrometry. A lack of knowledge of the desorption, plume transport, and analyte-ionization processes currently limits the reproducibility and optimization of the MALDI technique.

For the first time, gated laser-induced fluorescence (LIF) ICCD imaging, gas-phase optical absorption spectroscopy, and ion-current probe (IP) measurements have been employed to characterize plumes of desorbed products from 3-hydroxypicolinic acid (3-HPA) organic matrix crystals used in the MALDI technique.

Images of laser (193-nm and 248-nm) desorbed gas-phase matrix molecules were obtained using LIF from a time-delayed XeCl laser sheet [Fig. 1(a)]. Gas-phase absorption and emission spectra of the different regions in the images revealed that MALDI matrix plumes are dense and multicomponent in character and are composed primarily of intact matrix molecules propagating with nonthermal velocities, as shown in Fig. 1(b). Fragmentation, ionization, and acceleration can result from gas-phase absorption of the laser energy.

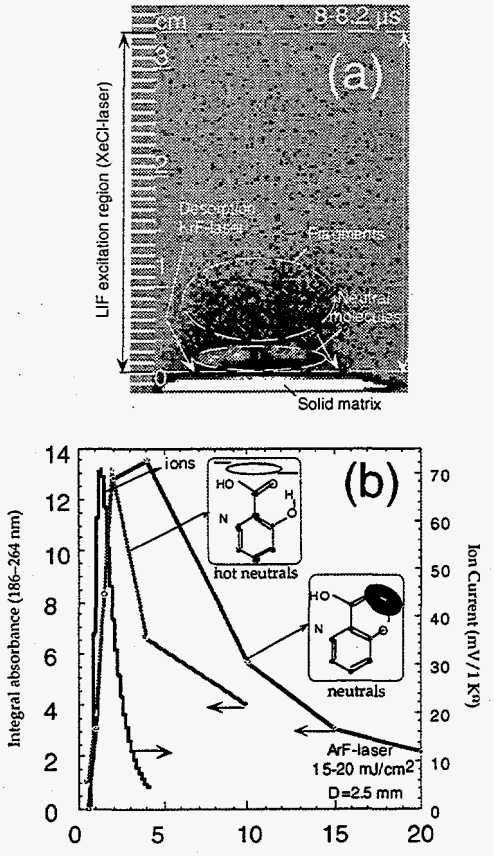

Fig. 1. (a) LIF image of desorbed 3-HPA neutral matrix molecules and fragments which were spectroscopically identified. (b) Time-of-flight curves (to d = 2.5 mm) showing the positions of ions, hot neutral, and neutral 3-HPA matrix molecules in the plume, as measured by ion probe and optical absorption spectroscopy.

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1. Summary of paper to be published.
2. ORNL/ORISE postdoctoral research associate.

MECHANISM FOR STRONG ADHESION OF COPPER FILMS DEPOSITED ONTO PULSED-LASER-IRRADIATED ALUMINA[1]

J.-W. Park,[2] A. J. Pedraza,[3] D. H. Lowndes, and W. R. Allen[4]

Reactions between deposited metals and oxide ceramic substrates are strongly restricted under thermodynamic equilibrium conditions. For example, pure Cu cannot reduce alumina (Al_2O_3) because the free energy of formation for Al_2O_3 (-377 kcal/mole) is much lower than for copper oxides. This frequent lack of reactivity leads to poor metal-ceramic bonding. However, it has recently been demonstrated that very strong adhesion (>70 MPa, suitable for industrial applications) can be produced if an Al_2O_3 substrate is first pulsed excimer laser irradiated either in an oxidizing or reducing atmosphere, followed by Cu film deposition and furnace annealing. The interfaces of strongly and weakly bonded Cu–Al_2O_3 couples were studied using Auger electron spectroscopy to determine the physical mechanism for the greatly enhanced adhesion.

Al_2O_3 substrates were irradiated with 10 excimer (308-nm) laser pulses in either air or (Ar–4% H_2) at 1 atm pressure. After sputter deposition of an 80-nm-thick Cu film, the Cu–Al_2O_3 specimens were vacuum annealed at 300° or 500°C for 1 h. A scanning Auger microprobe was used in combination with Ar ion sputtering to analyze the series of Cu-interface-Al_2O_3 structures.

It was found that a transitional layer was always present in Cu–Al_2O_3 couples that have high adhesion strength, while little or no transition region was present in weakly bonded couples or in the Auger spectra of couples deposited on unirradiated substrates and postannealed at 300°C. For substrates irradiated in air, ~30 MPa adhesion strength was produced by 300°C annealing, and >70 MPa was obtained at 500°C. For these specimens, the transitional region consisted of cuprous oxide close to the Cu film and a Cu-Al double oxide closer to the Al_2O_3 substrate. For substrates irradiated in Ar–4% H_2, annealing at 300°C produced only ~8 MPa adhesion strength but >70 MPa resulted from 500°C annealing. Transmission electron micros-copy observations revealed that for irradiations in either air or Ar–4% H_2, a metastable amorphous, substoichiometric near-surface alumina layer was formed.

It is concluded that the reaction of a Cu film with this metastable alumina layer during annealing to form a transitional layer of a Cu-Al-O double oxide interfacial compound is responsible for the greatly enhanced adhesion.

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1. Summary of paper: *Journal of Materials Research* (in press).
2. Graduate student from The University of Tennessee, Knoxville, Tenn.
3. The University of Tennessee, Knoxville, Tenn.
4. Y-12 Plant, Oak Ridge, Tenn.

NANOFABRICATION BY DIRECT EPITAXIAL GROWTH

G. Eres, F. Y. C. Hui,[1] T. G. Thundat,[2] and D. C. Joy[2]

The two main avenues for nanofabrication include adaptation of the existing device fabrication methods and self-assembly. Self-assembly is highly attractive conceptually, but in addition to its restricted application, controlling uniformity and spatial distribution of the features has been difficult. On the other hand, as feature sizes shrink and surface-to-volume ratios increase, the useful size of the structures fabricated by conventional methods become limited by the contamination and collateral damage caused by dry etching.

A novel, all dry approach that uses direct epitaxial growth to avoid the deleterious effects of etching in nanostructure fabrication is described. The two major requirements for achieving direct epitaxial growth are the ability to generate and subsequently to maintain and control spatial and chemical selectivity in the film-growth process.

The spatial selectivity is generated by patterning a surface hydride layer on silicon using a scanning electron beam. This artificially produced variation in surface reactivity is used as a template or a mask in subsequent epitaxy.

Chemical selectivity on the resulting pattern is controlled by supersonic molecular jet epitaxy which is a highly nonequilibrium film-growth method that uses translationally hot source gas species from a high-pressure gas expansion. Because the reactivity of the source gas molecules depends exponentially on the incident kinetic energy, the ability to tune the incident kinetic energy is utilized as a tool for controlling the selectivity of the film-growth process.

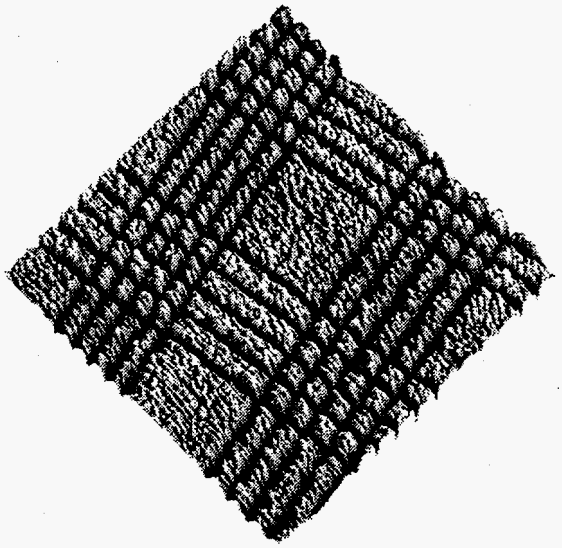

Fig. 1. AFM image of a Ge structure grown on Si(100). The line spacings (left to right) are 0.5 and 1 μm.

Arbitrary patterns with linewidths on the order of 0.1 μm have been achieved with Si, Ge, and SiC. An atomic force microscopy (AFM) image of a Ge structure grown on Si(100) is shown in Fig. 1. Systematic investigation of the effects of various patterning and growth parameters on spatial and chemical selectivity and their role in determining properties such as pattern resolution, pattern density, and aspect ratio are presently under way.

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1. ORNL/ORISE postdoctoral research associate.
2. Life Sciences Division, ORNL.
3. The University of Tennessee, Knoxville, Tenn.

SUPERSONIC MOLECULAR BEAM STUDIES OF THE DISSOCIATIVE CHEMISORPTION OF GeH_4 AND Ge_4H_6 ON THE Ge(100) AND Ge(lll) SURFACES[1]

G. Eres, M. E. Jones,[2] S. E. Roadman,[2] A. M. Lam,[2] and J. R. Engstrom[2]

The dissociative chemisorption of source gas molecules is the essential first step in thin-film growth from gaseous sources. Examination of the influence of molecular variables such as the incident kinetic energy and angle of incidence and macroscopic variables such as substrate temperature are essential for a better understanding of surface-limited thin-film growth reactions.

The reaction probabilities of GeH_4 and Ge_2H_6 on the Ge(100) and Ge(111) surfaces have been measured as a function of substrate temperature, incident kinetic energy, and angle of incidence employing supersonic molecular beam scattering techniques. At sufficiently large incident kinetic energies ($E_i > 1$ eV), both GeH_4 and Ge_2H_6 react by direct dissociative chemisorption on both surfaces examined, with the reaction probability increasing approximately exponentially with increasing (scaled) incident kinetic energy. At moderate kinetic energies ($E_i \sim 0.4$ eV), however, Ge_2H_6 reacts by a precursor-mediated mechanism on Ge(100) as demonstrated by a decrease in reaction probability with either increasing substrate temperature (Fig. 1) or incident kinetic energy. Interestingly, under similar conditions no evidence is found for precursor-mediated adsorption of Ge_2H_6 on the Ge(111) surface. The reaction of Ge_2H_6 does not exhibit a GeH_4 production channel on either Ge(100) or Ge(111) for the conditions examined.

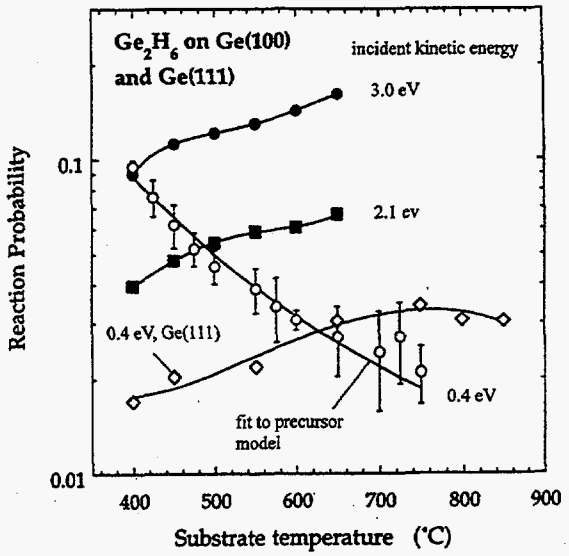

Fig. 1. Reaction probability of Ge_2H_6 on Ge(100) and Ge(111) as a function of substrate temperature.

The results obtained at high incident kinetic energies (>1 eV) are well described by a statistical model based upon a Rice-Ramsperger-Kassel-Marcus (RRKM) framework. The moderate incident kinetic energy results for Ge_2H_6 on Ge(100) are well described by a model that assumes reaction via a trapping, precursor-mediated mechanism.

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1. Summary of paper: *J. Chem. Phys.* 105, 7140 (1996).
2. Cornell University, Ithaca, N.Y.

TWO-MODULATOR GENERALIZED ELLIPSOMETER[1]

G. E. Jellison, Jr., and F. A. Modine

There is a growing need in industry to monitor and control film-growth processes in real time. However, many presently available in situ monitoring techniques are incompatible with gas-phase growth. In contrast, optical monitoring can be implemented for any transparent ambient. A two-modulator generalized ellipsometer (2-MGE) has been constructed to perform this task.

The 2-MGE consists of two polarizer-photoelastic modulator pairs acting as the polarization state generator (PSG) and as the polarization state detector (PSD), where the operating resonant frequencies of the two photoelastic modulators are significantly different. The detection system is designed to tune in on these frequencies, their harmonics, and to sum and difference frequencies.

The time-dependent intensity of the light incident upon the detector can be expressed as

$$I(t) = I_{dc} + I_{X0} X_0 + I_{Y0} Y_0 + I_{X1} X_1 + I_{Y1} Y_1 + I_{X0X1} X_0 X_1 + I_{X0Y1} X_0 Y_1 + I_{X0Y1} X_0 Y_1 + I_{Y0Y1} Y_0 Y_1$$

where

$$X_i = \sin[A_i \sin(w_i t)]$$

$$Y_i = \cos[(A_i \sin(w_i t))], i = 0, 1$$

The eight coefficients I_{X0}, I_{Y0}, etc., can be related directly to sample Mueller matrix elements, each normalized to the light intensity. Under normal circumstances, these eight coefficients are sufficient to characterize completely the reflection properties of the sample. This compares with standard spectroscopic ellipsometers, which measure two or three parameters.

The 2-MGE is particularly useful for samples that are anisotropic, either as thin-film or bulk materials. The instrument has been used to determine the ordinary and extraordinary complex refractive indices of a uniaxial bulk material (rutile, TiO_2) using only a single measurement. Other anisotropies measurable using the 2-MGE include out-of-plane strains and anisotropic surface and interfacial roughness.

Only two calibrations of the instrument are required. The first calibration characterizes the PSG and the PSD and does not need to be repeated. The second determines the azimuthal angles of the PSG and the PSD with respect to the sample.

A comparison of the capabilities of this instrument with commercially available instruments shows that the 2-MGE excels in several respects. It is possible to get a complete optical characterization of a sample surface with a single measurement, even if the sample is anisotropic. Traditional spectroscopic ellipsometers require at least three measurements. Other parameters of importance determined by the 2-MGE describe strain-induced retardation of vacuum chamber windows and sample depolarization effects.

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1. Summary of paper: *Applied Optics* (in press).

PARAMETERIZATION OF THE OPTICAL FUNCTIONS OF AMORPHOUS MATERIALS IN THE INTERBAND REGION[1]

G. E. Jellison, Jr., and F. A. Modine

The interpretation of optical measurements often requires a simple but accurate parameterized expression of the complex dielectric function $\varepsilon = \varepsilon_1 + i\varepsilon_2 = (n + ik)^2$ of materials as a function of energy. For example, the dielectric function of a thin film often depends upon deposition conditions and can be considerably different from that of the corresponding bulk material.

A new expression for the dielectric function of amorphous materials has been obtained using only five parameters. This formulation is obtained from the Tauc joint density of states multiplied by $\varepsilon_2(E)$ for a collection of noninteracting atoms determined by the standard quantum mechanical or Lorentz calculation and is given by:

$$\varepsilon_{2TL} = \frac{1}{E}\frac{AE_oC(E-E_g)^2}{(E^2-E_o^2)^2+C^2E^2} \qquad E \geq E_g$$

$$\varepsilon_{2TL} = 0 \qquad E \leq E_g$$

The peak transition energy is E_o, and C is the broadening term. The four fitting parameters are E_g, A, E_o, and C, and all are in units of energy. This model describes only interband transitions; any defect absorption, intraband absorption, or Urbach tail absorption will increase $\varepsilon_2(E)$ at lower energies. The corresponding real part of the dielectric function $\varepsilon_{1TL}(E)$ is determined by Kramers-Kronig integration, where an additional fitting parameter $\varepsilon_1(\infty)$ may be included; this integral can be evaluated in closed form.

The new expression for the dielectric function was fit to several n and k data sets found in the literature with E_g from 1.2 to 4.5 eV. Excellent fits to all the data sets were obtained. A graphical representation of the best fit to n and k of amorphous silicon is shown in Fig. 1.

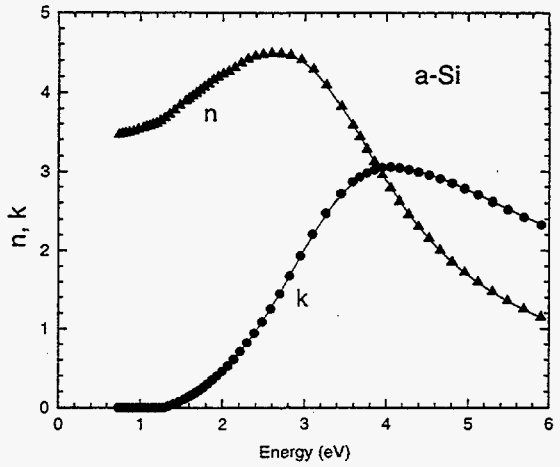

Fig. 1. Refractive index n and extinction coefficient k for amorphous silicon. The line shows the fit using the Tauc-Lorentz expression.

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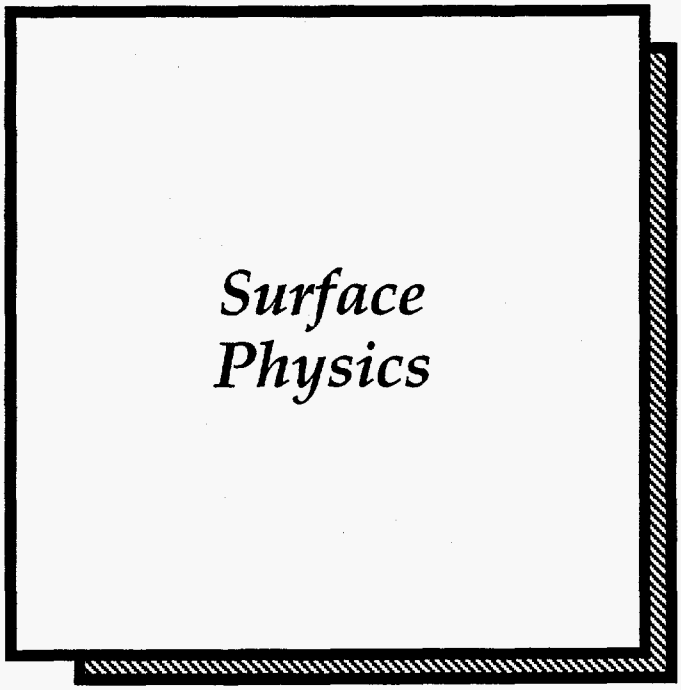
1. Summary of papers: *Appl. Phys. Lett.* **69**, 371 (1996); ibid, **69**, 2137 (1996).

Chapter 5

Structure of Solids and Surfaces


Surface
Physics

EVOLUTION OF MOUND MORPHOLOGY IN REVERSIBLE HOMOEPITAXY ON Cu(100)[1]

J.-K. Zuo[2] and J. F. Wendelken

Understanding the detailed mechanisms of thin-film growth becomes increasingly important as the length scales of electronic technology approach the nanoscale regime. While smooth films are usually desired, it is informative and useful to explore and exploit the "rough growth" nanoscale morphologies which are more commonly observed. Rough epitaxial growth results when atoms deposited on top of existing atomic height islands are inhibited from stepping down to a lower terrace by an edge diffusion barrier known as the Schwoebel barrier. On a (100) surface, the resulting three-dimensional growth takes the form of mounds with square pyramidal shapes. The pyramid sides exhibit a characteristic slope which is a function of an "uphill" current caused by repulsion of atoms arriving at an edge from above and the absorption of atoms arriving from below in competition with an opposing "downhill" current.

In this study, the evolution of mound separations and slopes has been studied at room temperature (RT) for Cu(100) where the growth is known to be reversible (i.e., atoms may evaporate from step edges making the structures unstable in time). The growth of mounds as a function of coverage was followed with both spot-profile analysis low-energy electron diffraction and scanning tunneling microscopy (STM). The mound separation shows coarsening vs. growth time with $L(t) \sim t^{1/4}$, as shown in Fig. 1. In addition, the mound slope reaches a final angle of ~5.6° following deposition of the equivalent of 100 atomic layers with a flux of 1-layer per minute at RT. Because the growth is reversible, the mound angle is a function of the deposition flux and temperature and decreases with time following the deposition. These results are consistent with a model in which the downhill current is driven by the line tension difference of successive mound step edges in balance with the uphill current.

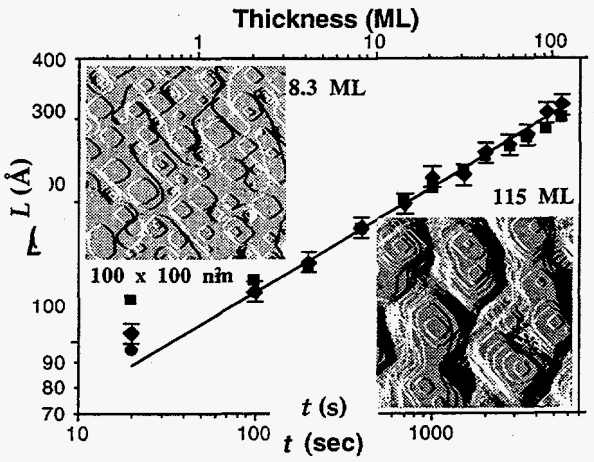


Fig. 1. Mound separation L vs. growth time t and thickness in monolayers (ML). STM images show mounds at coverages of 8.3 and 115 ML.

Previous studies of the detailed morphology of three-dimensional growth structures during homoepitaxy have been limited to cases where the growth is irreversible. However, growth is often reversible, and the resulting structures are unstable. This is the first study to explore and quantify the sources of this instability and its effect on thin-film growth.

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1. Summary of paper: *Phys. Rev. Lett.* 78, 2791 (1997).
2. Southwest Missouri State University, Springfield, Mo.

DIMER SHEAR AND FLUX-DEPENDENT SCALING IN Cu(100) HOMOEPITAXY[1]

A. K. Swan, Z.-P. Shi,[2] J. F. Wendelken, and Z. Y. Zhang

Diffusion of atoms and clusters on surfaces determines how two-dimensional (2D) island structures are formed. Because the morphology and distribution of the 2D islands may greatly influence the growth mode in the multilayer regime, it is important to identify the active atomistic processes in the early stages of island growth.

The dependence of the island distribution on the growth flux at a constant temperature of 213 K was studied with electron diffraction and scanning tunneling microscopy on a Cu(100) surface at a submonolayer coverage. For high to moderate flux, the island distribution followed the expected scaling law, indicative of irreversible aggregation (i.e., as soon as two adatoms meet on the surface, they stick together and the cluster can start to grow). As the flux is lowered further, the scaling of the island distribution changes drastically in a manner that suggests that clusters smaller than 9 atoms do not remain stable on the surface. Lowering the flux slows the clock rate of the system so that a kinetic pathway for dissociation becomes available for small clusters. Removing an atom from a compact cluster involves breaking two nearest neighbor (nn) bonds and is not likely to happen in the relevant time scale of the experiment [Fig. 1(a)]. To explain the low-flux results, a collective process where two atoms move together in a dimer shear mechanism in which only one net nn bond is broken was proposed. Subsequent dissociation may then proceed via single nn bond scission. Embedded atom calculations confirm that dimer shearing has a significantly lower energy barrier toward dissociation than double bond scission (Fig. 1). The expected time scale for dimer shear is consistent with the experimental time scale.

Previous studies of cluster dynamics have assumed that cluster dissociation and diffusion follows from sequential motion of individual atoms. Such processes cannot account for the results of this study. The proposed dimer shear mechanism not only provides a low-energy kinetic pathway for dissociation, it also explains the unexpectedly high diffusion rate of small clusters observed in several earlier experimental studies.[3]

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1. Summary of paper to be published.
2. ORNL/ORISE postdoctoral research associate.
3. Z.-P. Shi et al., *Phys. Rev. Lett.* **76**, 4927 (1996).

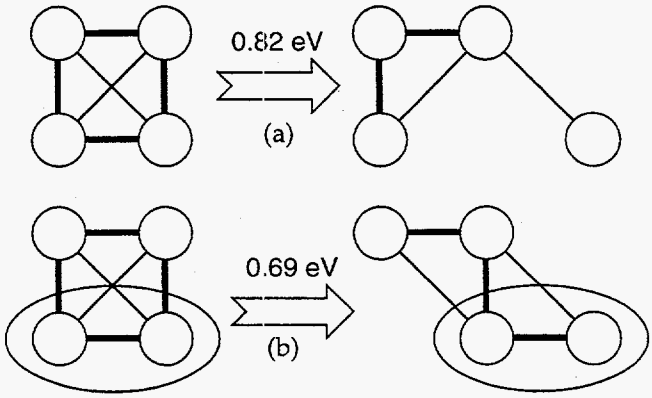

Fig. 1. Illustration of two different pathways toward diffusion/dissociation of small clusters. (a) sequential atom motion and (b) dimer shear.

DIFFUSION OF LARGE TWO-DIMENSIONAL ISLANDS ON Ag(100) AND Cu (100) SURFACES[1]

W. W. Pai,[2] A. K. Swan, J. F. Wendelken, and Z. Y. Zhang

Diffusion of large two-dimensional epitaxial islands on metal surfaces are driven by the random atomic motion of individual atoms. Theoretical studies have sought to establish a general scaling relation, $D \sim L^{-\alpha}$ between the diffusion coefficient of the island, D, and the island side length, L, where the value of α reflects the microscopic mechanism of the island mobility. Several different mechanisms can be operative causing different values of α. Simplified theories predict integer exponents for these processes, although noninteger exponents have been observed in detailed simulations. Hence, studies of the macroscopic island diffusion may yield significant information about the elementary atomistic processes involved in thin-film growth.

Here, the island motion, island coarsening, and island decay rates have been studied with scanning tunneling microscopy (STM) on Cu and Ag (100) surfaces. Movies assembled from the STM images immediately reveal that island coalescence due to island motion dominates the coarsening and that smaller islands move much faster than larger ones. Extensive quantitative measurements reveal the exact dependence of D vs. L (Fig. 1). The island decay was nonexistent on the Cu surface and very slight on Ag(100). Together with the results from coarsening measurements, the islands motion is shown to originate from atoms diffusing along the periphery of the islands. The noninteger exponent α is caused by the rate-limiting processes of detachment and attachment to edge kink sites.

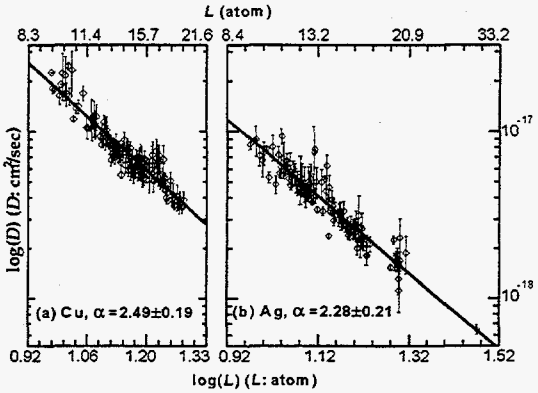

Fig. 1. Plot of island diffusivity vs. island length. (a) $\alpha = 2.49 \pm 0.19$, (b) $\alpha = 2.28 \pm 0.21$.

This work is the first comprehensive experimental study to elucidate the underlying atomistic mechanism for island diffusion. Simulations of various atomistic processes involved in thin-film growth can be stringently tested against our results. Furthermore, effective kinetic energy barriers could be experimentally determined by varying the temperature in this type of study. Finally, STM movies offer direct visualization of many dynamical phenomena. Combined with a thorough statistical analysis, it provides a powerful method capable of extracting significant information on atomic processes.

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1. Summary of papers to be published.
2. ORNL/ORISE postdoctoral research associate.

MANIPULATION OF MOLECULAR RADICALS AT ROOM TEMPERATURE[1]

W. W. Pai,[2] Z. Y. Zhang, J. Zhang,[3] and J. F. Wendelken

In addition to atomic scale imaging of surfaces, the scanning tunneling microscope (STM) may be used to manipulate atoms and molecules. While most such work has involved atoms on surfaces at cryogenic temperatures,[4] manipulation of molecules at room temperature has greater potential for application. Achieving this requires molecules with low surface thermal mobility which may be manipulated without rupture of intramolecular bonds. The only example published thus far involves the use of large molecules with flexibly attached functional groups.[5]

A conceptually different approach which utilizes small molecular radicals has been developed, with C_5H_5 (*Cp*) on Ag(100) as an example. Notably, the dynamics of the radicals can be directly visualized during manipulation, as shown in Fig. 1, revealing their preferred direction of motion to be perpendicular to the tip scan direction. The imaging of either the *Cp* or the track can be reversibly controlled by adjusting the tunneling resistance. As the tip scans from the bottom to the top, all *Cp* radicals are displaced upward, resulting in continuous tracks where each track represents the motion of a single *Cp*. Previously, atoms and molecules were individually moved parallel to the tip motion. At the gap resistance used in this work, the tip is estimated to be at least ~4–6 Å higher than the *Cp* plane. This suggests the force on the *Cp* is mainly perpendicular to the surface. As the tip is rastered across the scanned area, it first encounters one side of the *Cp*, tilting it, and causing it to diffuse in the tilt direction away from the tip. This diffusion occurs in discrete, or "quantized," jumps along the (110) directions always moving just ahead of the tip.

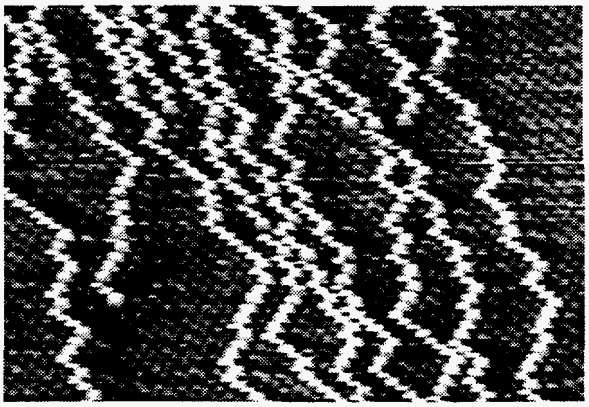

Fig. 1. Molecules in motion: The *Cp* radicals are manipulated using a STM at a gap resistance of ~266 MΩ. Each *Cp* radical appears as a single track with zigzag motions along the <110> directions. Image area: 15 × 10 nm². Scan direction is left to right.

The ability to manipulate small molecules or radicals at room temperature is novel and shows significant promise for nanofabrication. By manipulating radicals, it may be possible to study the reactivity of a single radical or even an artificial molecular assembly.

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1. Summary of paper to be published.
2. ORNL/ORISE postdoctoral research associate.
3. Postdoctoral research associate from The University of Tennessee, Knoxville, Tenn.
4. M. F. Crommie, C. P. Lutz, and D. M. Eigler, *Science* **262**, 218 (1993).
5. T. A. Jung et al., *Science* **271**, 181 (1996).

SURFACE CHARGE DENSITY WAVE TRANSITION IN THE ALPHA PHASE Sn OR Pb ON Ge(111)[1]

J. M. Carpinelli,[2] A. P. Baddorf, H. H. Weitering,[3] V. Jahns,[4] J. Zhang,[5] R. Stumpf,[6] and E. W. Plummer[7]

Minimization of a system's energy through loss of symmetry is pervasive in solid state physics and is the underlying mechanism for a variety of phenomena including Peierls distortions, the Jahn-Teller effect, spin density waves, and charge density waves. Although these mechanisms are inherently more important in systems with reduced dimensionality, this report documents the first clear example of a surface charge density wave (CDW) independent of bulk phenomena. These experimental and theoretical studies of the Ge(111)-($\sqrt{3} \times \sqrt{3}$)*R*30°-*M*-a interface, where *M* is either Pb or Sn, reveal that upon cooling below 255 K (Pb) or 215 K (Sn), the surface reversibly undergoes a symmetry reduction to a (3 × 3) periodicity. At the same time, electron energy loss spectroscopy reveals the opening of a gap in the electronic excitations of the surface, evidence for a metal-nonmetal transition at the surface. The valence electrons above and below a CDW transition are imaged directly using a variable-temperature scanning tunneling microscope (STM), as revealed in Fig. 1. Each white ball in the image represents valence electrons surrounding one Sn atom. At 90 K, clearly a new electron density distribution separates the atoms into two inequivalent types, in a 2:1 ratio. The influence of the CDW on the atomic positions was measured with surface x-ray diffraction using synchrotron radiation at the ORNL/UT/Exxon beam line at Brookhaven National Laboratory. Analysis reveals small displacements of 2/3 of the Sn atom cores, with associated response of the Ge substrate. The new symmetry of this surface CDW follows an energy decrease by interactions of valence electrons at nested (parallel) regions of the surface Fermi contour. This picture has been confirmed by first-principles local density approximation calculations for Pb, but has not yet been observed in theoretical calculations for Sn.

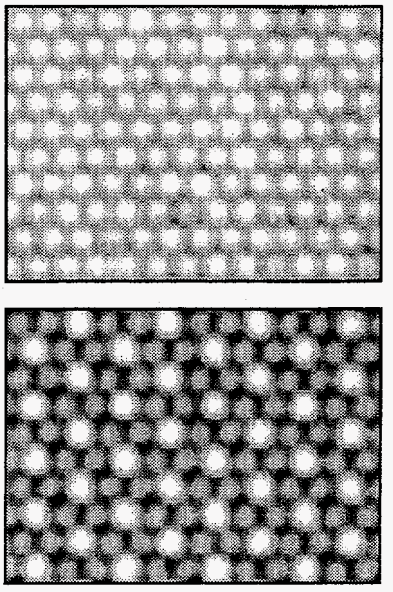

Fig. 1. STM topograph of Sn/Ge(111) at room temperature (upper panel) and at 90 K (lower panel). Between these temperatures, a reversible, two-dimensional phase transition occurs, producing a lower symmetry and new electron distribution.

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1. Summary of papers: *Nature* **381**, 398 (1996); to be published.
2. Graduate student from The University of Tennessee, Knoxville, Tenn. Present address: Sandia National Laboratories, Albuquerque, N. Mex.
3. Guest scientist from The University of Tennessee, Knoxville, Tenn.
4. ORNL/ORISE postdoctoral research associate.
5. Postdoctoral research associate from The University of Tennessee, Knoxville, Tenn.
6. Postdoctoral research associate from Sandia National Laboratories, Albuqueque, N. Mex.
7. ORNL/UT Distinguished Scientist.

DIRECT IMAGING OF THE TWO-DIMENSIONAL FERMI CONTOUR: FOURIER TRANSFORM SCANNING TUNNELING MICROSCOPY

P. T. Sprunger,[1,3] Ph. Hofmann,[2] L. Petersen,[1] E. Lægsgaard,[1] F. Besenbacher,[1]
B. G. Briner,[2] M. Doering,[2] H.-P. Rust,[2] A. M. Bradshaw,[2] and E. W. Plummer[4]

The Fermi surface of a metal is in many ways the epitome of modern solid state physics. Its shape is dictated by quantum mechanics, Fermi statistics for electrons, and the character of the Bloch states in the solid. Almost every physical observable is related in one way or the other to the shape of the Fermi surface. Due to an enhanced propensity for electronic instabilities, Fermiology-related issues are even more important in reduced dimensionality than three dimensions. The shape of the Fermi contour also dictates the wavelength of the Friedel charge oscillations that emanate from any imperfection in the surface. The Fourier transform (FT) of scanning tunneling microscopy (STM) images has been used to obtain a direct image of the Fermi contour. This technique[5] was demonstrated for the (0001) surface of Be where the two-dimensional Fermi contour is a circle. The most recent publication shows that the technique is applicable to complicated non-free-electron Fermi contours. Figure 1 (top) shows the calculated Fermi contour of the surface states for Be ($10\bar{1}0$). Figure 1 (bottom) is the FT of the STM image showing the Bragg Lattice spots and the elliptical Fermi surfaces.[6,7]

This technique offers many advantages compared with the conventional technique of angle-resolved photoemission. First, the energy resolution is limited only by kT; second, the momentum resolution is limited only by the windows of the experiment; third the bands can be mapped both above and below the Fermi energy in one experiment; and fourth, the experiment can be conducted in a magnetic field.

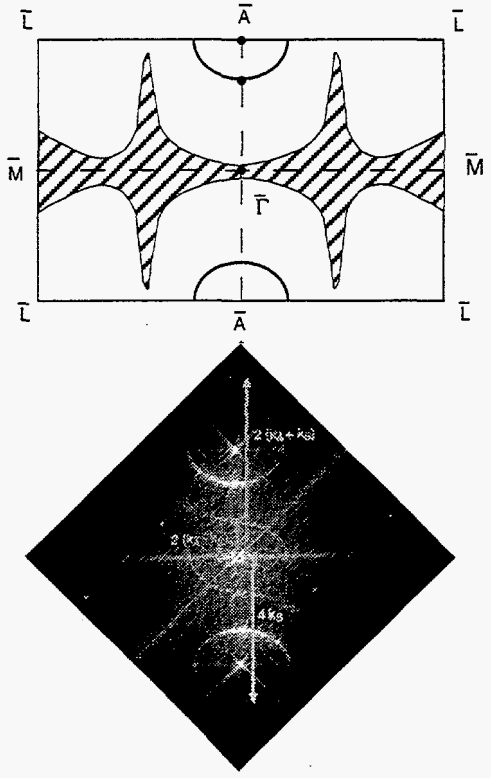

Fig. 1. Top is the theoretical Fermi contour of Be ($10\bar{1}0$), and the bottom figure is the Fourier transform of the STM image.

1. University of Aarhus, Aarhus, Denmark.
2. Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany.
3. Louisiana State University, Baton Rouge, La.
4. ORNL/UT Distinguished Scientist.
5. P. T. Sprunger et al., *Science* **275**, 1764 (1997).
6. Ph. Hofmann et al., *Physical Review Letters* (in press).
7. B. G. Briner et al., *Europhysics Letters* (in press).

LARGE THERMAL EXPANSION WITHOUT ANHARMONICITY OF BE(0001)

K. Pohl,[1] J.-H. Cho,[2] and E. W. Plummer[3]

It is well established that thermal expansion of a crystal is a direct manifestation of the anharmonic nature of the interatomic forces in solids. The reduction in coordination of atoms in the surface plane can be expected to increase the anharmonicity and consequently the thermal expansion of the interplanar spacing. Faced with the glaring discrepancy between first-principles calculations[4] and experiment[5] for the top-layer spacing of the close-packed Be(0001) surface (2.5% vs. 5.8%), the temperature dependence of the surface relaxation using low-energy electron diffraction (LEED) has been carefully measured. These data reveal two surprising results: (1) at 300 K, the Be(0001) top-layer expansion is +4.3% and not 5.8%, and (2) Be(0001) exhibits a large thermal expansion of the first interlayer spacing even though high-resolution electron energy loss spectroscopy shows no enhancement in the surface anharmonicity.[6] The top-layer spacing expands from +3.1% at 110 K, +4.3% at 300 K, to +6.7% at 700 K resulting in a thermal expansion coefficient of 70×10^{-6} K^{-1}, six times the bulk value. In addition, the rms vibrational amplitudes of the surface atoms are a factor of 2 to 3 larger than the bulk. Figure 1 shows the change in the surface relaxation with temperature. The reason for this deviation (+4.3% vs. +5.8%) from the previously reported room temperature expansion lies in the improved treatment of thermal vibrations at surfaces, a crucial ingredient in LEED theory for surfaces with very different dynamical properties than the bulk.

In stark contrast to the general understanding, thermal expansion is not the result of anharmonicity in the interlayer potential; instead, it results from the broken symmetry at the surface and special electronic properties of the Be surface. Recent local density approximation (LDA) calculations have reproduced the observed temperature effects on the Be(0001) surface relaxation; their results are displayed in Fig. 1. The theory suggests that a softening of the in-plane vibrations leads to the enhanced surface expansion, while the interlayer potential in their LDA calculation shows only very small anharmonic contributions. This is evidence for new physics of anharmonic phenomena and has to be understood.

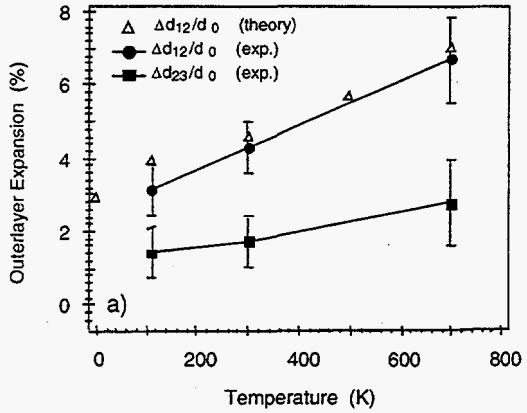

Fig. 1. Change in the surface relaxation as a function of temperature from experiment (filled) and theory (open).

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1. Graduate student from the University of Pennsylvania, Philadelphia, Pa.
2. ORNL/ORISE postdoctoral research associate.
3. UT/ORNL Distinguished Scientist.
4. R. Stumpf et al., *Phys. Rev. B* **51**, 13748 (1995).
5. H. L. Davis et al., *Phys. Rev. Lett.* **68**, 2632 (1992).
6. J. B. Hannon, Ph.D. thesis, University of Pennsylvania (1994).

HYDROGEN ON (110) SURFACES OF Mo_x AND $MoRe_{(1-x)}$ ALLOYS: MECHANISM FOR THE GIANT PHONON ANOMALY[1]

M. Okada,[1] A. P. Baddorf, D. M. Zehner, and E. W. Plummer[2]

Despite several structural differences, H-saturated Mo(110) and W(110) surfaces each exhibit a giant phonon anomaly which was not well understood following extensive investigations with a wide variety of surface science techniques.[4,5] Two possible origins of the giant phonon anomaly have been reported. It could be a Kohn anomaly where electron-hole pairs, with a momentum vector which spans two nesting lines of the Fermi surface, are coupled to surface phonons. An alternate proposal for the origin of the anomaly involves disorder of H, following evidence of a "liquid-like" state in vibrational spectra for H on the W(110) surface.[5]

The clean- and H-covered (110) surfaces of Mo and closely related alloys of Mo and Re, where small quantities of Re randomly replace Mo atoms, retaining the same crystal structure have been studied. Nuclear reaction analysis was used to determine absolute coverages of deuterium (chemically equivalent to H), which for the saturated surfaces of both Mo(110) and $Mo_{0.95}Re_{0.05}$(110) is 1 monolayer. The symmetry of the surface structures, observed with low-energy electron diffraction, is (2×2) for 1/2 monolayer and (1×1) for the saturated surfaces. Vibrations measured with high-resolution electron energy loss spectroscopy indicate H prefers to bond in quasitrigonal sites. For both pure Mo and $MoMo_xRe_{(1-x)}$(110) alloy surfaces, the vibrations are discrete, ruling out disorder, and providing strong evidence that the "liquid-like" state of H/W(110) is not related to the giant phonon anomaly. The Fermi contour (Fig. 1) has been painstakingly measured for H-saturated $Mo_{0.95}Re_{0.05}$(110); that is, the values of momentum to which the occupied electron bands are filled, using angle-resolved ultraviolet photoemission spectroscopy at the UT/ORNL beam line at Brookhaven National Laboratory (U-12). Results of this study support interpretation of the anomaly as nesting (i.e., Kohn type) and identify regions involved in the nesting with good agreement with phonon data.

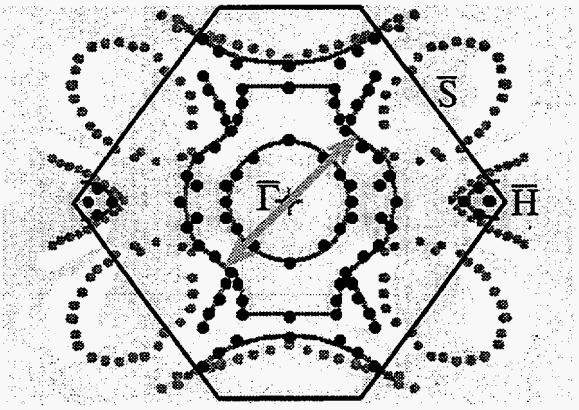

Fig. 1. Experimentally determined Fermi contour for H-saturated $Mo_{0.95}Re_{0.05}$(110) (dark dots) and Mo(110) (gray dots).[6] Shaded areas are projections of the bulk Fermi surface. Nesting is indicated by the diagonal arrow.

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1. Summary of papers: *Surf. Sci.* **363**, 416 (1996); *Surf. Sci.* **373**, 145 (1997).
2. Guest scientist from the University of Tokyo, Rpppongi, Japan.
3. ORNL/UT Distinguished Scientist.
4. E. Hulpke and J. Lüdecke, *Phys. Rev. Lett.* **68**, 2846 (1992).
5. M. Balden et al., *Phys. Rev. Lett.* **73**, 854 (1994).
6. R. H. Gaylord, K. H. Jeong, and S. D. Kevan, *Phys. Rev. Lett.* **62**, 2036 (1989).

REDUCTION IN STRUCTURAL RIPPLING BY HYDROGEN ADSORPTION ON NiAl(110)[1]

A. T. Hanbicki,[2] H. L. Davis,[3] A. P. Baddorf, D. B. Poker, E. W. Plummer,[4] B. Hammer,[5] and M. Scheffler[6]

The interaction of hydrogen with the NiAl(110) surface is a prototypical adsorbate-bimetallic alloy system. NiAl(110) maintains the bulk stoichiometry and has two components; each surface constituent, however, has very different chemical properties. On the clean surface, the Ni and Al atoms are not coplanar, as they are in the bulk. Instead, a vertical rippling results from the reduction of the Al(*p*) - Ni(*d*) hybridization at the surface because of loss of nearest neighbors.

In general, elemental metals with filled *d*-bands exhibit a dissociative barrier to the H_2 molecule. This has been found to be true also on the NiAl(110) surface, where the *d*-bands are also full. Predissociated hydrogen (formed by flowing H_2 over a hot filament) readily bonds to the surface, up to an coverage of 1 ML. Absolute coverages were determined from nuclear reaction analysis at the Surface Modification and Characterization Research Center at ORNL.

The effect of H chemisorption on the NiAl(110) surface structure was determined independently by low-energy electron diffraction intensity-voltage (LEED *I-V*) and x-ray diffraction (XRD) measurements. Results for the clean (a) and H-covered (b) surfaces are shown in Fig. 1. Lines show contours of a quality of fit parameter between LEED *I-V* data and calculation. For the clean surface, the outermost layer spacing relative to the bulk is Δd_{12} (Ni) = -3.95% and Δd_{12}(Al) = +5.45%. The magnitude of the ripple is 9.4% or 0.19 Å. For the H-saturated surface, Δd_{12} (Ni) = -3.05% and Δd_{12} (Al) = +2.3%, corresponding to a ripple of 5.35% or 0.11 Å. Results from a state-of-the-art first-principles theory are also indicated in Fig. 1. Reasonable agreement is found for the clean surface structure. H does reduce the magnitude of the surface ripple but does not remove it as suggested by theory.

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1. Summary of papers: *Surf. Sci.* **365**, L639 (1996) and *Surf. Sci.* **331**, 811 (1995).
2. Graduate student from the University of Pennsylvania, Philadelphia, Pa.
3. ORNL retiree.
4. ORNL/UT Distinguished Scientist.
5. University of Pennsylvania, Philadelphia, Pa.
6. Fritz-Haber-Institut, Berlin-Dahlem, Germany.

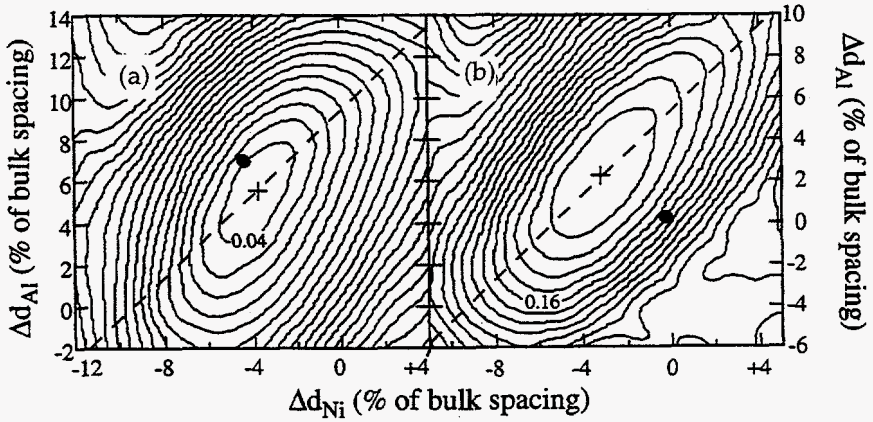

Fig. 1. Contour plot of quality of agreement, indicating Ni and Al outerlayer spacings for clean (a) and H-saturated (b) experiments (+) and theory (●).

MOTT INSULATING GROUND STATE ON A TRIANGULAR SURFACE LATTICE[1]

H. H. Weitering,[2] X. Shi,[3] P. D. Johnson,[4] N. J. DiNardo,[5] and K. Kempa[6]

Alkali-metal/silicon interfaces are model systems for testing theoretical models of bonding, metallization, and electronic transport in systems of reduced dimensionality.

The electronic properties of a monatomic alkali layer on the Si(111):B surface have been investigated with photoemission spectroscopy and inverse photoemission spectroscopy (PES/IPES). By combining PES and IPES, the energy needed to spatially separate an electron and a hole (i.e., the conductivity gap) can be deduced. Momentum-resolved spectra in Fig. 1 show that the surface state band of K/Si(111):B is split into two dispersionless subbands S_1 and S_2. The centroids of the bands are separated by ~1.1 eV. This indicates that the alkali layer is a correlated insulator or Mott insulator with an on-site correlation energy U of ~1.1 eV. However, the conductivity gap is much smaller (~0.1 eV) as the tails of the broad subbands nearly overlap.

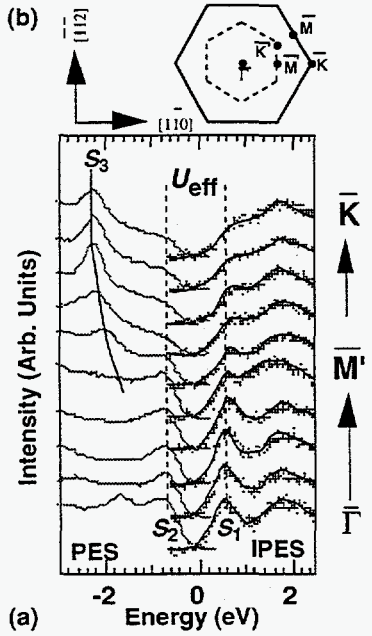

Fig. 1. PES/IPES data of K/Si(111):B.

The large linewidths are likely due to the Franck-Condon broadening of the positive and negative ion final states in the PES/IPES experiment. By incorporating the Hubbard U into a simple force constant model, the observed line widths can be accounted for quantitatively. It is concluded that the lateral conduction mechanism is of the polaron type where U is largely compensated by a local lattice relaxation during a charge excitation.

This interface possibly represents a novel model system for the spin 1/2 Heisenberg antiferromagnet on a triangular lattice. So far, theory has not been able to predict with certainty whether or not this "frustrated" spin lattice exhibits long-range ordering. The next challenge is to measure the magnetic susceptibility of this model spin system using a highly sensitive magnetic probe.

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1. Summary of paper: *Phys. Rev. Lett.* **78**, 1331 (1997).
2. Guest scientist from The University of Tennessee, Knoxville, Tenn.
3. Postdoctoral research associate from The University of Tennessee, Knoxville, Tenn.
4. Brookhaven National Laboratory, Upton, N.Y.
5. Drexel University, Philadelphia, Pa.
6. Boston College, Chestnut Hill, Mass.

DO *p*-BONDED SILICON CHAINS DIMERIZE?[1]

H. H. Weitering,[2] X. Shi,[3] S. C. Erwin,[4] and K. Kempa[5]

The Si(111) 3 × 1-Li surface reconstruction is a beautiful example of a quasi-one-dimensional Si lattice. The essential building block is a *p*-bonded polyacetylene-like chain of Si atoms. It is not yet clear, however, how these chains are backbonded to the Si substrate. Two structural models are currently debated: the extended Pandey model, introduced by Erwin, and the Seiwatz model, by Weitering et al.

The surface state band structure of the three-domain Si(111) 3 × 1-Li reconstruction has been measured with angle-resolved photoemission spectroscopy (ARPES). The ARPES data are totally inconsistent with the calculated dispersions of the extended Pandey model. Calculations for the Seiwatz model, however, are consistent with the data along the *p*-bonded chain direction (G-A-K) only (Fig. 1). A possible explanation for the remaining discrepancy is that the *p*-bonded chains actually dimerize rather than buckle as predicted. The following observation seems to support this idea.

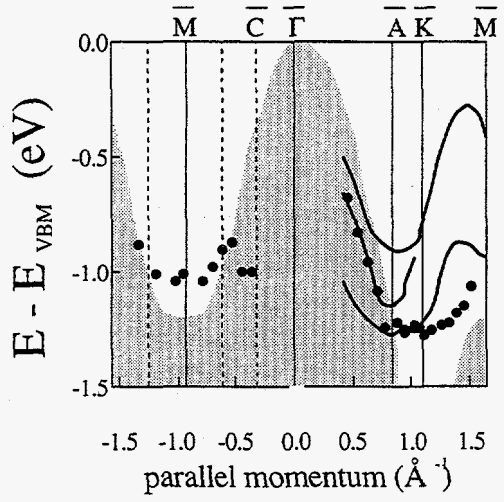

Fig. 1. Calculated dispersions for the Seiwatz model and experimental data points.

Scanning tunneling microscopy studies of the closely related Si(111) 3 × 1-Ag surface show an intriguing "dimer-switch" from the (3 × 1) into the (6 × 1) reconstruction which was apparently caused by the tip-surface interaction.[6] The dynamics of this switch likely involve the propagation of a soliton in the dimerized or conjugated Si chains. Evidently, Si dimers in neighboring chains "communicate" as they rearrange themselves into a (6 × 1) superlattice. Taking Coulomb interactions as the dominant interaction between *p*-electrons in neighboring Si chains, an annealing process using classical Monte Carlo methods was simulated. The (3 × 1) structure turns out to be the most stable phase when alkali metals mediate the chain-chain interaction, but (6 × 1) is most stable for metals containing *d*-orbitals. This provides an explanation for the "electrostatically enforced" switch from metastable (3 × 1) into stable (6 × 1) for Si(111)-Ag.

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1. Summary of papers: *Phys. Rev. B* **54**, 10585 (1996); *Physica B* (in press).
2. Guest scientist from The University of Tennessee, Knoxville, Tenn.
3. Postdoctoral research associate from The University of Tennessee, Knoxville, Tenn.
4. Naval Research Laboratory, Washington, D.C.
5. Boston College, Chestnut Hill, Mass.
6. J. M. Carpinelli and H. H. Weitering, *Surf. Sci.* **331**, 1015 (1995).

COLLECTIVE EXCITATIONS IN THIN K FILMS ON Al(111)

B.-O. Kim[1] and E. W. Plummer[2]

The electronic excitations in thin metallic overlayers have attracted interest for nearly three decades because of the wide range of available electron densities and film thicknesses. Nevertheless, the understanding of these modes is far less complete than that of clean simple metals. Experimental verification of the Jellium-based theoretical calculations,[3] which predicted a richer set of features for thin films than for clean surfaces because of the interference between the substrate-film and film-vacuum interfaces, has been reported.[3]

Photoyield and electron energy loss spectroscopy (EELS) measurements were combined to elucidate the nature of the collective electronic modes of thin K films on Al(111). Figure 1 shows the observation of the new adsorbate-induced excitations at $q_{||} = 0$ using the photoyield measurement. They correspond to the antisymmetric slab mode and the multipole surface plasmon. With increasing coverage, the overlayer excitations turn into the collective modes of semi-infinite K.

The transition of these modes for $q_{||} > 0$ were also observed using EELS. At finite $q_{||}$, these modes undergo a transition toward the K multipole and monopole surface plasmons. Figure 2 shows the negative dispersion of the multipole mode which supports the existence of a hybridization gap in the overlayer excitation spectrum arising from the avoided crossing of the principal bulk-like overlayer mode and the adsorbate multipole surface plasmon.

In conclusion, using both EELS and surface photoemission, a systematic understanding of the collective electronic excitations in thin K films on Al(111) has been achieved. It has been found that the photoyield and EELS data are consistent and that the observed dispersions are in good agreement with the predictions based on the time-dependent local density approximation.

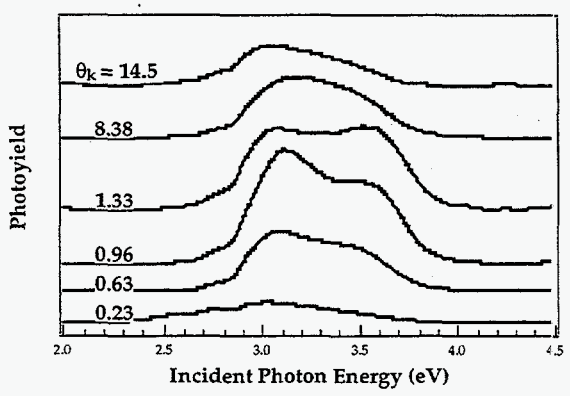

Fig. 1. Measured *p*-polarized photoyield spectra of thin K films adsorbed on Al(111).[4]

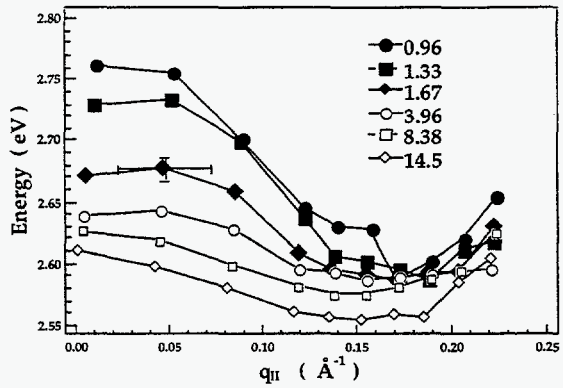

Fig. 2. Measured momentum dispersion of main collective mode of K on Al(111) for various coverages.[4]

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1. Graduate student from the University of Pennsylvania, Philadelphia, Pa.
2. UT/ORNL Distinguished Scientist.
3. A. Liebsch, *Phys. Rev. Lett.* **67**, 2858 (1991).
4. B. Kim, E. W. Plummer, and A. Liebsch, submitted to *Physical Review Letters*.

Electron Microscopy

EXPERIMENTAL OBSERVATION OF ARSENIC AT SILICON GRAIN BOUNDARIES[1]

M. F. Chisholm and S. J. Pennycook

Interfaces such as grain boundaries (GB) play critical roles in determining the physical properties of complex materials and structures. Impurity segregation in interfaces and grain boundaries often alters these properties in dramatic ways. In this report, atomic-resolution Z-contrast images show that As impurities segregate to particular atomic columns in a Si grain boundary.

Figure 1(a) is a Z-contrast image of a symmetric tilt boundary doped with arsenic revealing periodic bright features. The extra intensity corresponds, on average, to an extra 5 at.% As in each bright triangular feature. These features are parts of mixed dislocation cores identified as 2 or its mirrored core, 2', in the derived boundary structure presented in Fig. 1(b). Thus, the image indicates that arsenic not only substitutes for silicon in a few selected sites in this boundary but that it also selects just one of the two mixed dislocation cores in the boundary (two of the six dislocations in each period of the GB). These consistently bright features are not observed in the undoped bicrystal.

The compositional sensitivity of the image is extremely high. It is estimated that there is a thickness of the order of 20 nm in this section of the sample, corresponding to approximately 40 atoms per column. With an As concentration of 5% in the selected column, there are, on average, only two arsenic atoms per column. This small number of impurity atoms explains the variability in the intensities from individual columns.

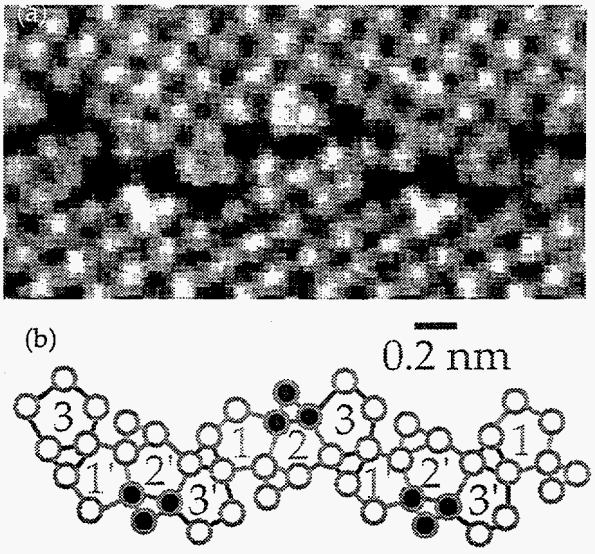

Fig. 1. (a) Z-contrast image of a symmetric 23° ⟨001⟩ tilt boundary in Si that has been doped with arsenic. The extra intensity seen at particular sites in the boundary indicates As segregates to special sites in the host interface without otherwise changing the boundary structure. (b) Schematic of the projected atomic column positions of the boundary core, obtained directly from the image, showing the three dislocations that form the boundary. The highlighted column positions in the schematic correspond to bright features in the image.

1. Summary of paper to be published.

ATOMIC STRUCTURE OF A SYMMETRIC 27°[001] TILT GRAIN BOUNDARY IN MgO[1]

Y. Yan,[2] M. F. Chisholm, G. Duscher,[3] and S. J. Pennycook

Grain boundaries determine the chemical, mechanical, and electrical properties in polycrystalline materials. It is of fundamental importance to understand grain boundary behavior at the atomic scale.

The atomic structure of a symmetric 27°[001] tilt grain boundary in MgO has been determined by high-resolution Z-contrast imaging and simultaneous electron energy loss spectroscopy (EELS) using a 300-kV VG HB603U scanning transmission electron microscope with a 1.3-Å probe. The atomic configuration in the grain boundary core is found to be considerably less open than the structures proposed earlier for similar materials.

Figure 1 shows the Z-contrast image of the grain boundary and the projected structure derived from the image. It is clearly seen that the boundary is a shared plane of atoms with the same atomic column density as a bulk crystal {100} plane. The boundary consists of an array of separated perfect-edge dislocation cores with Burgers vector $\mathbf{b} = \mathbf{a}\langle 100\rangle$. It is interesting to point out that the spacing between dislocation cores in the boundary is not uniform. The arrangement, which follows the Fibonacci sequence, can be accurately predicted. These dislocation cores, labeled A, B, and C in the schematic, are composed of seven atomic columns. However, the intensity from the central column is significantly reduced relative to its neighbors, indicating the possibility of reduced atomic density at the center of the cores. It is also noted that certain columns in the boundary (3 and 5 in the schematic) are brighter than their neighbors. This implies that impurity segregation of elements with atomic numbers greater than that of Mg (Z = 12) should be considered. High spatial resolution EELS analysis has found that the segregated atoms are Ca. It may be that it is the impurities that have stabilized this structure; *ab initio* calculations are in progress.

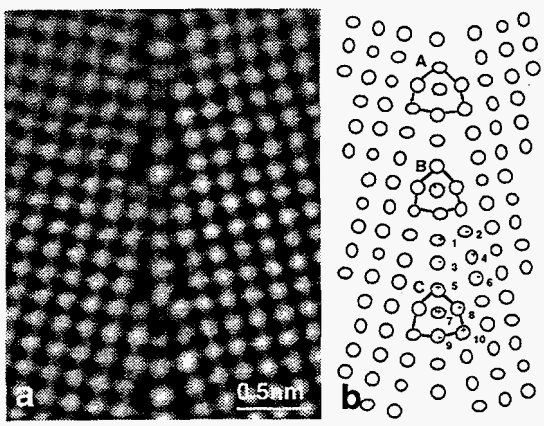

Fig. 1. (a) High-resolution Z-contrast image of a symmetric 27°[001] grain boundary in MgO and (b) the boundary structure derived from the image.

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1. Abstract of paper to be published.
2. ORNL/ORISE postdoctoral research associate.
3. Joint postdoctoral research associate: ORNL/ORISE and the University of Illinois at Chicago, Chicago, Ill.

INCOHERENT ATOMIC-STRUCTURE IMAGING: THE DYNAMICAL OBJECT FUNCTION

P. D. Nellist[1] *and S. J. Pennycook*

A Bloch wave analysis has shown rigorously how a large detector in a scanning transmission electron microscope leads to an incoherent image. Rather than a perturbative treatment,[2] all beams falling on the detector in a new reciprocal space formulation were included.

The key advantage of the new formulation is that it includes analytically the degree of coherence between different Bloch waves $\phi^{(j)}$ and $\phi^{(k)}$ for a specific detector geometry D_{ADF} through the coherence parameter:

$$C_{jk}(\mathbf{K}_i) = \sum_{\mathbf{g}} D_{\mathbf{g}}^{ADF} \Phi_{\mathbf{g}}^{(j)}(\mathbf{K}_i) \Phi_{\mathbf{g}}^{(k)*}(\mathbf{K}_i)$$

The remarkable role of the detector geometry is revealed by Fig 1. Although 311 Bloch states are included in the calculation, the image is dominated by only two, the most tightly bound 1s-type Bloch states on the In and As columns. Calculation of images is therefore enormously simplified.

Furthermore, at the limit of high detection angles, the $C_{jj}(\mathbf{K}_i)$ terms are proportional to the expectation value of transverse kinetic energy squared, which can be related to the square of the projected potential. Therefore, the electron equivalent of incoherent imaging described first by Lord Rayleigh[3] was achieved, and the chemical sensitivity observed experimentally was also explained. Incoherent images are directly invertible and effectively overcome the phase problem of electron diffraction.

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1. ORNL/ORISE postdoctoral research associate. Present address: Cavendish Laboratory, Cambridge, U. K.
2. S. J. Pennycook and D. E. Jesson, *Phys. Rev. Lett.* **64**, 938 (1990).
3. Lord Rayleigh, *Phil. Mag.* **42**, 167 (1996).

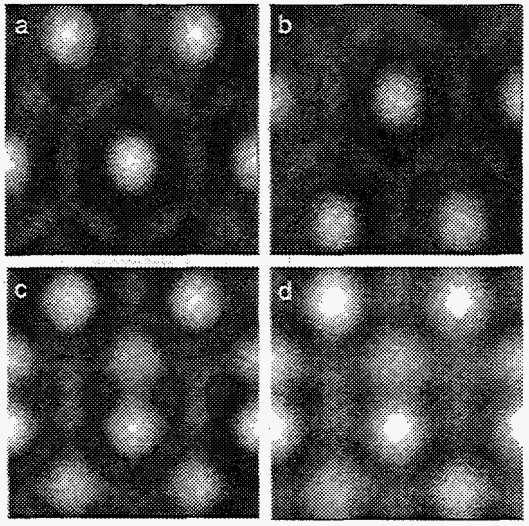

Fig. 1. Bloch states contributing to the image for InAs<110> at 300 kV at the limit of high specimen thickness and 25-mrad detector inner radius (a) In 1s state, (b) As 1s state, (c) In and As 1s states, and (d) the sum over all 311 states in the calculation, which adds only a constant background to the image.

DIRECT IMAGING OF THE ATOMIC CONFIGURATION OF ULTRADISPERSED CATALYSTS[1]

P. D. Nellist[2] and S. J. Pennycook

Direct observation of the atomic dispersion of a catalytic metal on its support material is essential for the understanding of catalytic activity and degradation mechanisms. Here, it is achieved for the first time through Z-contrast imaging in a 300-kV scanning transmission electron microscope. Individual platinum and rhodium atoms ultradispersed on γ-Al_2O_3 supports are imaged directly and their preferred configurations determined. Conventional transmission electron microscopy is not sensitive to features this small; scanning tunneling microscopy cannot be used because of the highly insulating support.

Platinum and rhodium showed clear differences in their interaction with the support. In Fig. 1(a), a sample of ultradispersed 3 wt.% Pt on γ-Al_2O_3 individual Pt atoms are resolved, showing that some clusters actually contain as few as two Pt atoms. The larger bright features are three-dimensional structures that are unresolved because they are not aligned accurately in the beam direction. By measuring the atomic spacings and angles using maximum entropy analysis, the Pt atoms were found to be constrained to match the substrate lattice parameters [Fig. 1(b)].

A very different behavior was seen for 1.2 wt.% Rh on the same substrate. The Rh atoms agglomerated in the form of a thin raft, only one or two atoms thick. Such differences in the atomic structure and morphology of ultradispersed catalysts are now able to be revealed and correlated with their catalytic performance.

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1. Summary of paper: *Science* **274**, 413 (1996).
2. ORNL/ORISE postdoctoral research associate. Present address: Cavendish Laboratory, Cambridge, U. K.

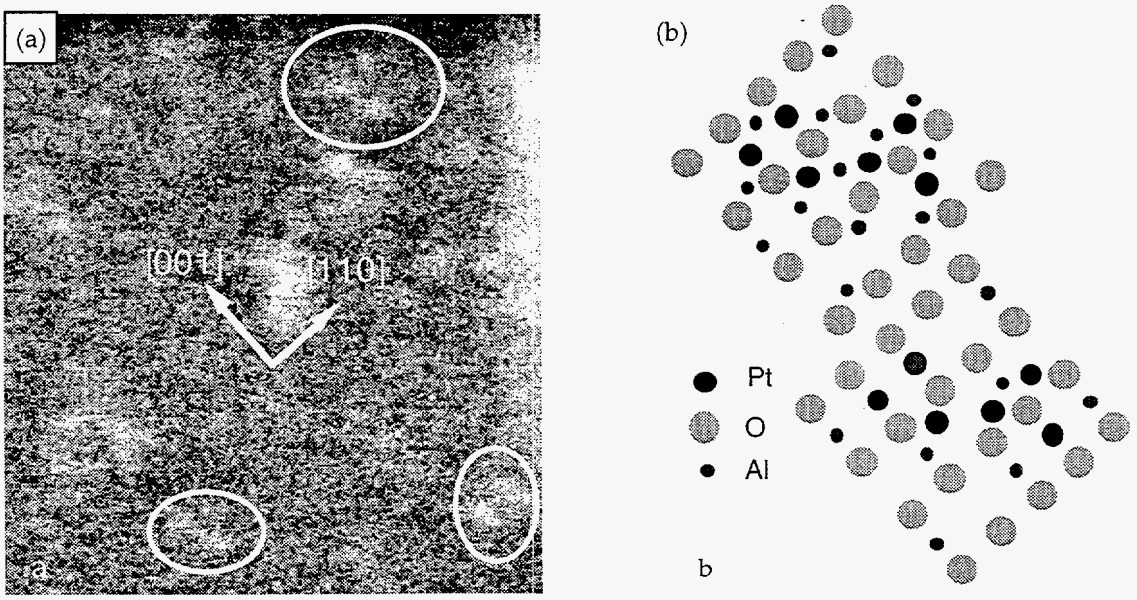

Fig. 1. (a) Z-contrast image of small Pt clusters on γ-Al_2O_3. Circled are examples where individual Pt atoms form dimers and trimers. (b) Schematic showing the two (110) surfaces possible for γ-Al_2O_3 with possible Pt configurations.

ATOMIC-SCALE STRUCTURE AND CHEMISTRY OF CERAMIC/METAL INTERFACES[1]

M. F. Chisholm, D. A. Shashkov,[2] and D. N. Seidman[2]

Dispersion-hardened alloys, metal-matrix fiber-reinforced composite materials, oxide films and coatings on the surface of high-temperature alloys, and microelectronic packaging are important examples of ceramic metal composites that play a significant role in modern materials technology. It is widely recognized that to design and to control materials properties, a fundamental understanding of the atomic-scale structure and chemistry of ceramic/metal (C/M) interfaces is necessary.

In this study, internal oxidation of ternary metallic alloys was used to examine solute segregation at C/M interfaces. It was found that the resulting {222}MgO/Cu(Ag) interfaces are generally flat, with some double and quadruple-height steps, particularly near the corners of a precipitate. The Z-contrast image of the Cu/MgO interface (Fig. 1) shows Ag segregated to the interface and located just inside the MgO precipitate rather than in the Cu matrix. The observed image intensities are consistent with the 0.2 monolayer of Ag found in the interface region using atom-probe field-ion microscopy and electron energy loss spectroscopy. It was also found that the spacing between the last plane of the oxide (containing Ag) and the first Cu plane is 0.268 nm, 10% larger than the {111} spacing in MgO and 28% larger than the {111} spacing in Cu. This totally unexpected result is presently the basis of a new theoretical study of Ag segregation to the {222}MgO/Cu interface.

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1. Summary of paper to be published.
2. Northwestern University, Evanston, Ill.

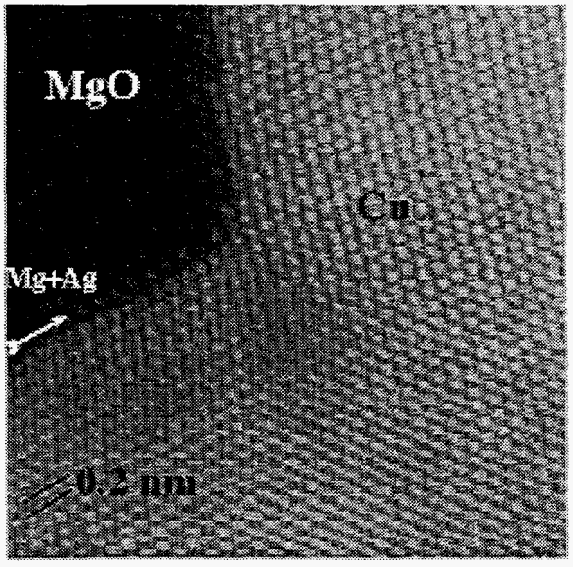

Fig. 1. Z-contrast image of the corner of a MgO precipitate in Cu. The first metal plane of the oxide is distinctly brighter than the others indicating that the 0.2 monolayer of Ag known to have segregated to this interface is located primarily in this plane.

LOCAL PROPERTIES OF BSCCO—Ag-SHEATHED TAPES BY STEM

C. Prouteau,[1] G. Duscher,[1] S. J. Pennycook, and N. D. Browning[2]

The most highly developed HTSC material for power applications is the $(Bi/Pb)_2Sr_2Ca_2Cu_3O_{10}$ (Bi-2223) silver-sheathed multifilamentary tapes which are now produced with critical current densities over 3×10^4 A/cm^2 at 77 K. To interpret the experiments related to dissipation mechanism, the local atomic and electronic structures of the grain boundaries have to be studied.

The cross section of such a wire has been investigated in a scanning transmission electron microscope (STEM) HB501. The electron energy loss spectroscopy (EELS) spectra presented in Fig. 1 have been recorded at a high-angle grain boundary and in the bulk material from an area about 1.5 × 2 nm. The copper-L2,3 edge of the bulk spectra indicates that the average valence of copper in the bulk is between II and III as it is supposed to be in the HTSC cuprates. A shift of the copper-L2,3 edge at the grain boundary indicates that the copper valence is less than 1. This result may partially account for the low critical current density (J_c) of this tape.

The first Z-contrast image of this kind of tape presented in Fig. 2 exhibits a dislocation core at a low-angle grain boundary. The bright fringes correspond to the lead/bismuth planes. Their periodicity (≈31 Å) corresponds to the *c* parameter of the Bi-2212 phase. These low-angle grain boundaries do not appear to be responsible for the low J_c, but the presence of the Bi-2212 phase itself is detrimental to superconductivity.[3]

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1. Joint postdoctoral research associate: ORNL/ORISE and the University of Illinois at Chicago, Chicago, Ill.
2. University of Illinois at Chicago, Chicago, Ill.
3. B. Hensel et al., *Phys. Rev. B* **51**, 5456 (1995).

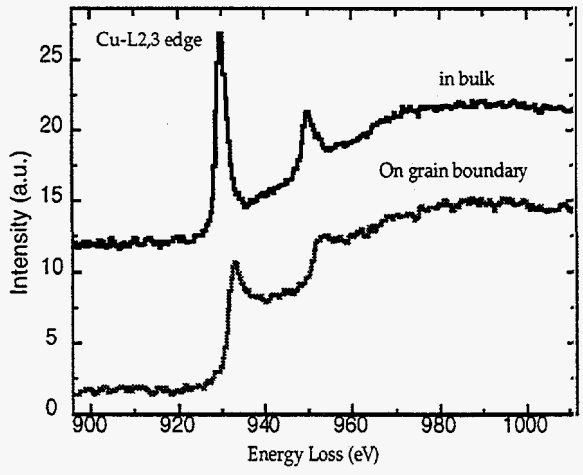

Fig . 1. Energy loss near-edge structure copper-L2,3 edge at a high-angle grain boundary in BSCCO tape.

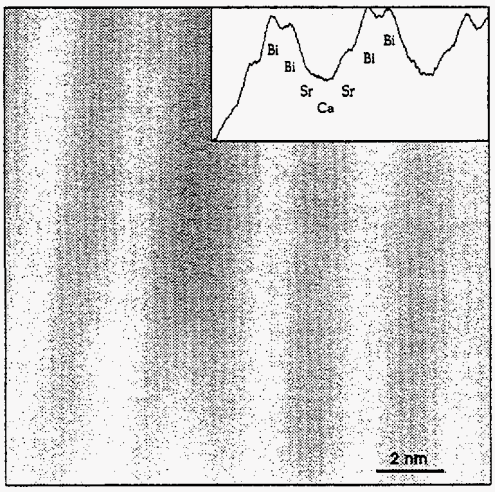

Fig. 2. High-resolution Z-contrast image of a dislocation core at a low-angle grain boundary in Bi-2212 (insert: plot of the intensity).

ATOMIC STRUCTURE OF Si-SiO_2 INTERFACE

G. Duscher,[1] F. Banhard,[2] H. Müllejans,[2] M. Rühle,[2] and S. J. Pennycook

Investigations of the atomic structure of Si-SiO_2 interfaces have mostly been performed with high-resolution transmission electron microscopy. However, the interpretation of the phase contrast in the amorphous phase at the interface is not unique. While Ourmazd et al.[3] suggested a crystalline phase at the Si-SiO_2 interface, Akatsu and Ohdomari[4] attributed the same contrast to interface roughness parallel to the incident electrons.

Z-contrast imaging (Fig. 1) reveals that there is no crystalline SiO_2 at the interface. The interface electron energy loss spectroscopy (EELS) ionization edge shows a similar energy loss near-edge structure (ELNES) at both interfaces. The intensity of the first peak is reduced at the interface, as expected for silicon-rich oxide. The shift of the second peak, compared with SiO_2, is related to a widening of the SiO_4^{4+} tetrahedra. The only difference between the spectra of both the interfaces is the slight shift in energy of the first peak of the oxygen K edge ELNES.

Interpreting this in terms of Si–O bond angles suggests a model shown schematically in Fig. 2. The SiO_4^{4+} tetrahedra are positioned on top of a silicon atom with a bond angle of about 180°, much higher than in stochiometric SiO_2. The combination of *Z*-contrast imaging and EELS studies excludes the possibility of three-dimensional ordering at the interface. Furthermore, the atomic structure is revealed to be a one-dimensional ordering of the SiO_4^{4+} tetrahedra. Experiments in progress with *Z*-contrast imaging should verify the proposed atomic model.

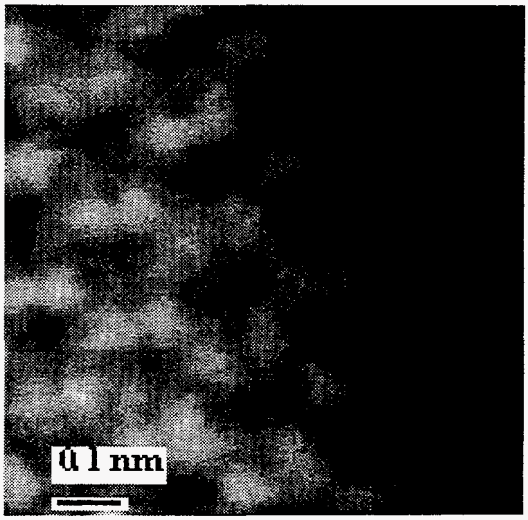

Fig. 1. *Z*-contrast image of Si-SiO_2 interface

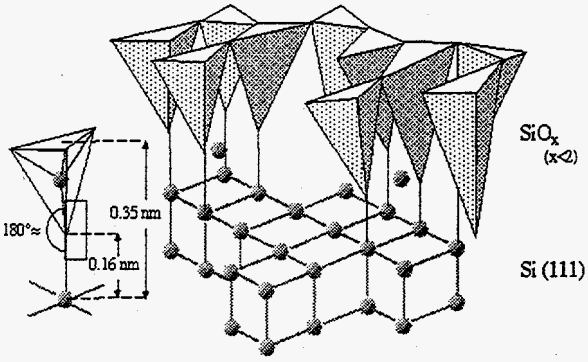

Fig. 2. Schematic atomic structure model of the Si-SiO_2 interface

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1. Joint postdoctoral research associate: ORNL/ORISE and the University of Illinois at Chicago, Chicago, Ill.
2. MPI für Metallforschung, Stuttgart, Germany.
3. A. Ourmazd et al., *Phys. Rev. Lett.* **59**, 213 (1987).
4. H. Akatsu and I. Ohdomari, *Appl. Surf. Sci.* **41–42**, 357 (1989).

MICROSTRUCTURAL STUDY OF CdTe GROWN ON (001)Si BY MOLECULAR BEAM EPITAXY

Y. Xin,[1] *N. D. Browning,*[2] *and S. J. Pennycook*

Compound II–VI semiconductors, such as CdTe and HgCdTe, have many applications (e.g., infrared detection). Consequently, there have been intense efforts to grow CdTe and HgCdTe on Si substrates.[3] Understanding the growth mechanism of CdTe on (001)Si is critical for controlling device properties. Figure 1(a) is a plan view showing the initial growth of CdTe, and Fig. 1(b) shows a cross section of the subsequent growth of a thick layer.

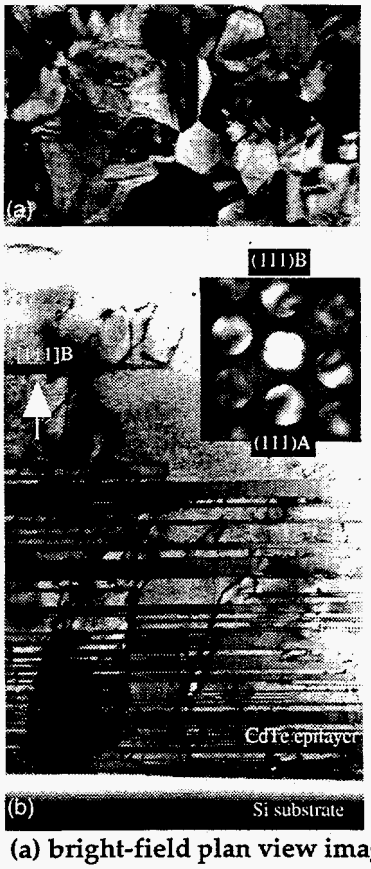

Fig. 1. (a) bright-field plan view image of a thin CdTe layer showing many small domains at the initial growth stage; (b) bright-field cross-sectional image showing the lamellae twins in the CdTe layer and twin-free region with inset showing CBED pattern, indicating the Te-terminated orientation.

There has been much confusion over the polarity of the CdTe layer [i.e., whether the epilayer is Te-terminated ([111]B) or Cd-terminated ([111]A)]. Several methods have been used to determine the polarity [i.e., chemical etching, convergent beam electron diffraction (CBED), and high-resolution Z-contrast imaging]. The polarity of the thick CdTe epilayer appears to be Te-terminated determined by CBED and chemical etching. However, high-resolution Z-contrast imaging[4] has shown the opposite polarity at the initial growth stage.

It is, therefore, suggested that at the initial growth stage, three-dimensional islands (or domains) are formed with a size of around 100 nm. As growth proceeds, the growth planes with Te-termination grow faster and overgrow the Cd-terminated grains to form a good quality CdTe layer. Future work using high-resolution Z-contrast imaging on a scanning transmission electron microscope HB603 with probe size 1.2 Å will be carried out to confirm the proposed growth mechanism.

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1. Joint postdoctoral research associate: ORNL/ORISE and the University of Illinois at Chicago, Chicago, Ill.

2. University of Illinois at Chicago, Chicago, Ill.

3. Y. P. Chen et al., *J. Electron. Mater.* **24**, 475 (1995).

4. D. J. Wallis, unpublished result.

AB INITIO DENSITY-OF-STATES (DOS) CALCULATIONS FOR Ti AND Ti OXIDES

G. Duscher,[1] S. Köstlmeier,[2] C. Elsässer,[2] and S. J. Pennycook

Electron energy-loss spectroscopy (EELS) is a powerful tool to determine not only the chemistry but also the electronic and atomic structure at grain boundaries by analyzing the energy-loss near-edge structure (ELNES). However, the interpretation of ELNES has previously been mostly qualitative.

Density functional theory is used in the local density approximation with norm-conserving pseudopotentials for the (frozen) cores and a mixed basis of plane waves and atom-centered functions for the valence electrons. The mixed basis provides the advantage to be efficient, especially for strongly attractive ionic pseudopotentials such as oxygen or transition metals.

Results are obtained for bulk titanium (hcp) and TiO_2 (rutile). The calculated DOS of all available edges (O-K, Ti-K, and Ti-L of TiO_2 in Fig. 1) show a very good agreement to experimental data.[3] The location and the overall shape of the peaks are well reproduced. This is not only one of the best agreements between experimental and theoretical ELNES of K-edges so far, but also the ELNES of L-edges can be calculated accurately with this method for the first time.

This mixed-basis pseudopotential method shows good promise for calculations of the structure and DOS at grain boundaries in the future.

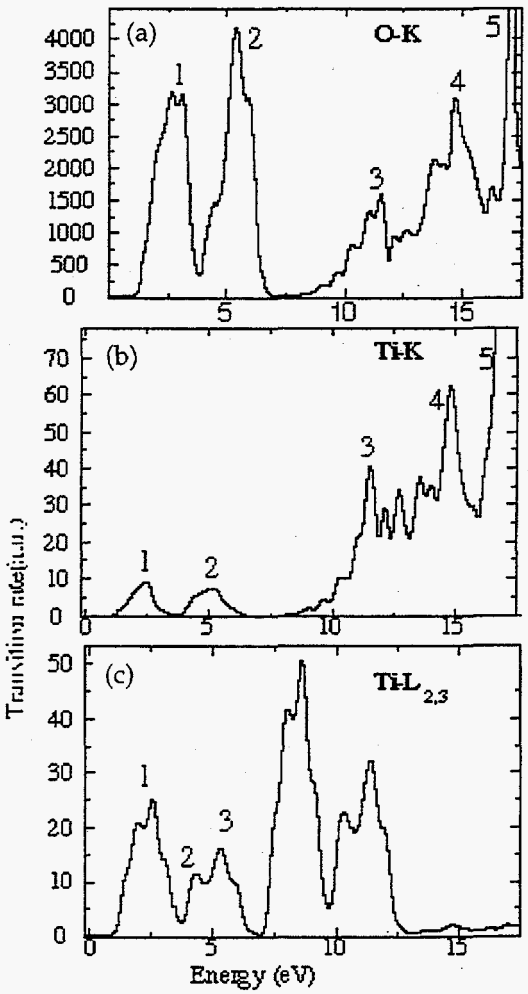

Fig. 1. Momentum and site-resolved DOS of TiO_2 (rutile).

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1. Joint postdoctoral research associate: ORNL/ORISE and the University of Illinois at Chicago, Chicago, Ill.
2. MPI für Metallforschung, Stuttgart, Germany.
3. Brydson et al., *Ultramicroscopy* **59**, 81 (1996).

MORPHOLOGICAL EVOLUTION OF STRAINED FILMS BY COOPERATIVE NUCLEATION[1]

D. E. Jesson, K. M. Chen,[2] S. J. Pennycook, T. Thundat,[3] and R. J. Warmack[3]

The morphological evolution of stressed solids is a central issue in many important areas of materials science including fracture, phase transformations, and epitaxial growth. Most recently, strain-induced islanding of semiconductor films has been used to fabricate devices with enormous potential such as the quantum dot laser. Therefore, it is essential to understand the physics of island formation to optimize conditions for the growth of quantum dots.

Conventionally, strain-driven roughening has been viewed as an Asaro-Tiller-Grinfeld (ATG) instability.[4,5] In this model, no energy barrier exists to roughening so one would anticipate a gradual increase in the amplitude of the roughness across extended regions of the film. Indeed, this is apparently confirmed by the frequent appearance of surface ripples during the growth of semiconductor films.

The ripple formation process has been investigated by the controlled in situ annealing of $Si_{0.5}Ge_{0.5}$ thin films. Surprisingly, atomic force microscopy (Fig. 1) reveals that the ripple forms by a cooperative nucleation process involving islands and pits. Islands nucleate adjacent to pits and then pits nucleate next to islands as the ripple spreads laterally across the film to form a continuous morphology. This mechanism of ripple growth differs from the conventional view of ripple formation as an ATG instability and can be attributed to the elastic interaction of islands and pits which provides energetically favorable nucleation sites.[1] Most importantly, combined with further annealing, cooperative nucleation is a potentially useful means of manipulating microstructures on the mesoscopic scale to form high-density quantum dot arrays.

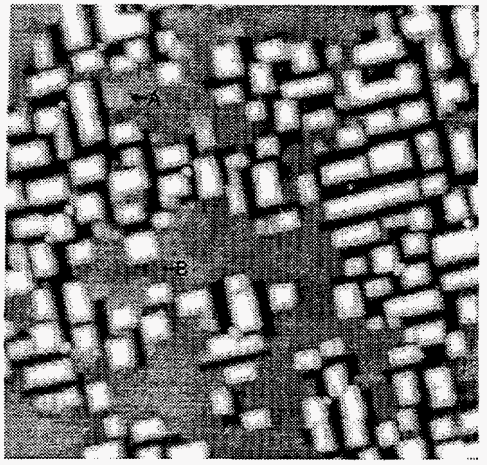

Fig. 1. Atomic force microscopy image of a 5-nm thick $Si_{0.5}Ge_{0.5}$ alloy layer grown on Si(001) and annealed for 5 min. at 550°C. This image reveals cooperative nucleation of discontinuous surface ripple domains where islands and pits nucleate adjacent to each other as indicated.

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1. Summary of paper: *Phys. Rev. Lett.* **77**, 1330 (1996).
2. ORNL/ORISE postdoctoral research associate.
3. Life Sciences Research Division, ORNL.
4. R. J. Asaro and W. A. Tiller, *Metall. Trans.* **3**, 1789 (1972).
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SELF-LIMITING GROWTH AND SHAPE INSTABILITY OF STRAINED FACETED ISLANDS[1]

D. E. Jesson, G. Chen,[2] K. M. Chen,[2] S. J. Pennycook, T. Thundat,[3] and R. J. Warmack[3]

Mechanisms of facet formation and growth have long been outstanding issues in surface physics and materials science. In particular, faceting governs many key processes including crystal growth and etching. Recently, it has been discovered that facets also play a central role in the growth of coherently strained semiconductor islands. Although this can profoundly influence the control of island sizes for the fabrication of quantum dot devices, insight into facet growth mechanisms has been extremely limited.

Islands typically assume a pyramidal geometry as shown in Fig 1. The island is essentially relaxed at the peak but strongly compressed at the base due to the mismatch strain in the film. This variation in strain has been calculated using finite element calculations and used as the basis of a model for the growth of an embryo on the facet surface. The calculation reveals the existence of an energy barrier to complete the facet. Physically, the barrier is linked to the stress concentration which occurs at the base of the island. The effect of this stress concentration (and hence the energy barrier) increases as the island gets larger, producing self-limiting growth. This effect has been confirmed experimentally by atomic force microscopy (AFM) measurements which show that the growth rate of large islands decreases dramatically. This identifies a very useful characteristic of strained facets which can be utilized to control island-size distributions.

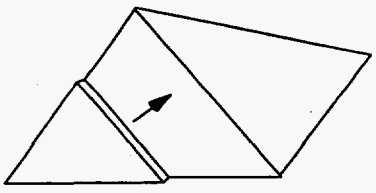

Fig 1. Schematic illustration of the model used to investigate strained facet growth. An embryo expands from the bottom left-hand corner to cover the facet surface.

A stunning consequence of the facet growth mechanism is the prediction that the pyramidal shape can be kinetically unstable to elongation. The resulting "hut shapes" arise due to an increase in the stress concentration associated with the longer side of a slightly perturbed (elongated) square-based pyramid, resulting in a shape instability. This insight explains a significant mystery of strained-layer epitaxy; namely, why hut clusters arise.[4] It also shows that because elongated shapes result from kinetics, lower energy square-based shapes can be obtained by annealing. This has been confirmed directly by AFM and has important implications for the fabrication of quantum dots.

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1. Summary of paper to be published.
2. ORNL/ORISE postdoctoral research associate.
3. Life Sciences Research Division, ORNL.
4. Y.-W. Mo et al., *Phys. Rev. Lett.* **65**, 1020 (1990).

MAPPING SURFACE STRAIN USING SCANNING TRANSMISSION ELECTRON MICROSCOPY[1]

D. E. Jesson, M. F. Chisholm, and S. J. Pennycook

The transition of a planar-stressed film to an island morphology is often accompanied by significant local bending of atomic columns in the near-surface region. Surface strains are of considerable interest because they control the morphological development of thin films which is relevant to the fabrication of quantum dot arrays. A new method of surface strain imaging has been developed using scanning transmission electron microscopy (STEM) which provides a directly interpretable image of columnar bending.

A surface strain image of $Si_{0.5}Ge_{0.5}$ quantum dots is shown in Fig 1. The image is formed by scanning a defocused STEM probe across the surface of a specimen and then collecting transmitted electrons using a large inner-angle annular detector. The contrast is linked to the excitation of *s*-type Bloch waves which is very sensitive to the local orientation of the column at the surface of the film. Changes in *s*-state channeling can be linked directly to boundary matching of the incident electron probe wave function at the entrance surface. This lends itself to a particularly simple optical interpretation of the contrast in terms of the alignment of the crystal columns with the incident rays of the probe. The sign of the defocus then immediately indicates the sense of curvature of the distorted columns. Additionally, only one side of the specimen contributes strongly to the contrast, so that image interpretation is straight forward. It is envisaged that this new technique for mapping surface strain will provide important new information for the study of strained microstructures.

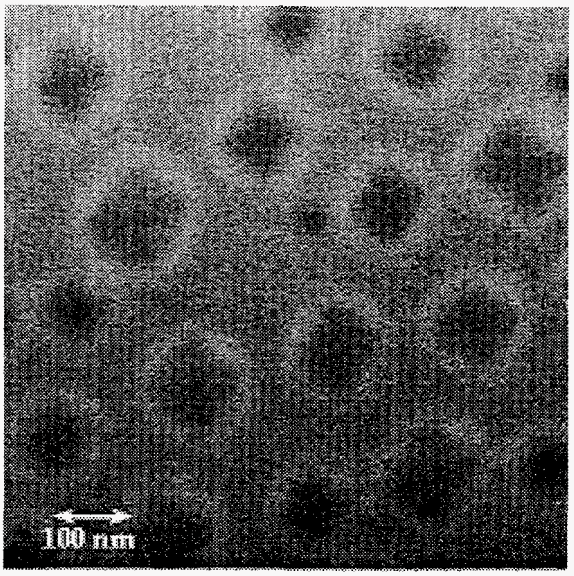

Fig 1. Surface strain image of $Si_{0.5}Ge_{0.5}$ quantum dots. The image was obtained in an overfocus condition so that the dots appear darker than the planar film due to the outward curvature of the atomic columns. The bright region surrounding the dots is a convolution effect.

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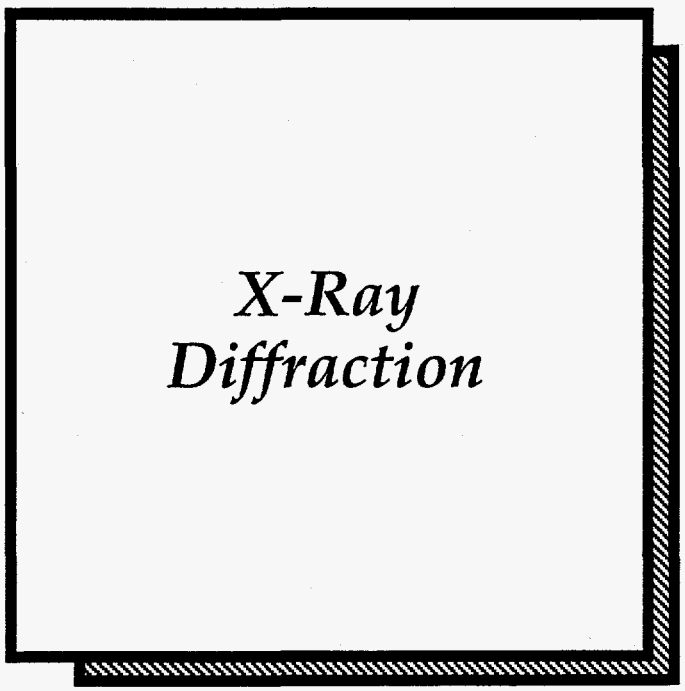
1. Summary of paper to be published.


X-Ray
Diffraction

INELASTIC X-RAY SCATTERING MEASUREMENT OF THE MANY-BODY LOCAL-FIELD FACTOR IN ALUMINUM[1]

B. C. Larson, J. Z. Tischler, A. Fleszar,[2] and A. G. Equiluz[3]

Electron-electron interactions play a fundamental role in determining the physical properties of metals, including optical, transport, and magnetic phenomena. The random-phase approximation has long provided an excellent theoretical description of *long-range* collective electronic interactions in terms of plasmons. However, despite their fundamental importance and four decades of intense theoretical effort, *short-range* exchange-correlation effects are neither well understood, nor has it been possible to explore these effects experimentally.

The first experimental insight into these short-range effects in a simple metal—Al—has been observed. Large wave-vector inelastic x-ray scattering measurements have been made on the X-14 beam line at the National Synchrotron Light Source, with energy resolution of 2.4 eV. These measurements have been analyzed using *ab initio* dynamical electronic response calculations[1] (including the actual band structure) to determine both the wave vector q and energy dependence ω of the so-called many-body local-field factor (LFF), $G(q,\omega)$, which characterizes the short-range interactions.

As shown in Fig. 1, the LFF values in the critical large wave-vector (~2-k_F) regime are significantly larger than predicted by available theoretical calculations. On the other hand, it is important to notice that the LFF values measured at lower wave vectors (i.e., below ~1.5 k_F) are in good agreement with nearly all theoretical predictions. The agreement at the lower wave vectors resolves a long-standing discrepancy between electron energy loss measurements of the LFF and many-body theory and is a direct result of the inclusion of band structure in the electronic response analyses.[1,4] The large wave vector results emphasize the fact that short-range exchange-correlation effects are not well understood, even in so-called simple metals such as Al.

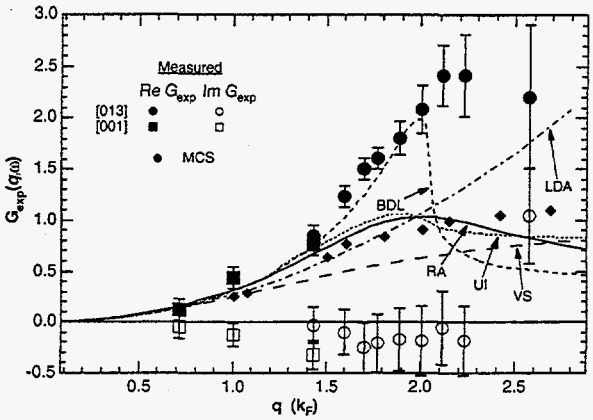


Fig. 1. Comparison of measured and calculated LFF values as a function of wave vector in units of the Fermi wave vector. The solid circles (and squares) and the open circles (and squares) are the real and imaginary parts, respectively. The theoretical LFF values represent static calculations (see Ref. 1).

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1. Summary of paper: *Phys. Rev. Lett.* **77**, 1346 (1996).
2. University of Würtzburg, Germany.
3. ORNL/UT Collaborative Scientist.
4. A. A. Quong and A. G. Eguiluz, *Phys. Rev. Lett.* **70**, 3955 (1993).

IMPACT OF BAND STRUCTURE AND MANY-BODY EFFECTS ON THE ELECTRONIC RESPONSE OF NEARLY FREE ELECTRON METALS

B. C. Larson, J. Z. Tischler, A. Fleszar,[1] and A. G. Eguiluz[2]

Combined inelastic x-ray scattering and first-principles dynamical response calculations have demonstrated that band-structure effects in electronic energy loss spectra are much more pervasive than generally realized. High-resolution x-ray scattering measurements (~0.75 eV) made on Al using the X-21 beam line at NSLS have shown that band-structure effects have a significant impact on the energy loss spectrum of Al at both small and large wave vectors. In addition to the well-known band structure and many-body local-field factor (LFF) plasmon energy shifts, zone-boundary collective state resonances, spectral shifts to lower energies, and high-energy tails are observed at all wave vectors.

Figure 1 compares calculated noninteracting polarizabilities, $\chi^o(q,\omega)$, for jellium and band electrons. As mentioned above, the band calculations contain a sharp dip at ~8 eV, an overall spectral shift to lower energies, and a high-energy tail; none of these are present in the jellium calculations. The zone-boundary collective state structures (generated by energy gaps at the Brillouin zone boundary) are well known; however, the spectral shift to lower energies and the tail in the dynamical electronic response calculations at high energies are actually of greater importance for quantitative analyses of the shape of energy loss spectra in terms of many-body local-field effects.

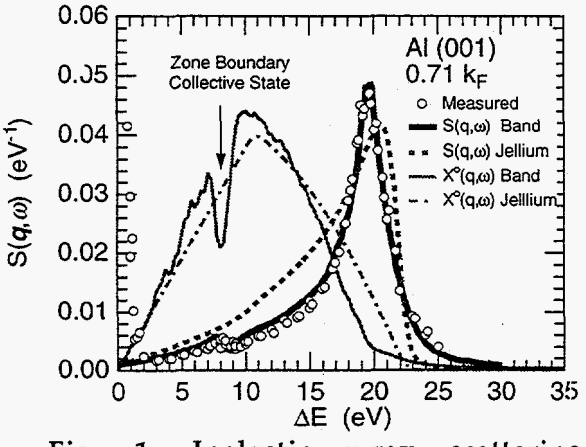

Fig. 1. Inelastic x-ray scattering measurements for Al at a wave vector of 0.71 k_F. Jellium model $\chi^o(q,\omega)$ and $S(q,\omega)$ calculations are compared with measurements and first-principles calculations, including band structure. The (complex) LFF values for $S(q,\omega)$ are (0.5, 0.044) for jellium and (0.2, 0.09) for band calculations.

The dynamical structure factor calculations, $S(q,\omega)$, in Fig. 1 show that response calculations, including band structure, are in remarkably good agreement with the measured loss spectrum at a wave vector of 0.71 k_F. This is in contrast to the poor agreement of the jellium calculations with the measurements.

The effects discussed above relate to diagonal contributions to the dielectric matrix. Measurements along the [001] direction have demonstrated the impact of off-diagonal effects as well through the interaction[3] of the band structure induced folded plasmons with single-particle continuum states.

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1. University of Würzburg, Würzburg, Germany.

2. UT/ORNL Collaborative Scientist.

3. K. Sturm, W. Schülke, and J. R. Schmitz, *Phys. Rev. Lett.* **68**, 228 (1992).

EPITAXIAL YBaCuO FILMS ON ROLL-TEXTURED METAL SUBSTRATES

J. D. Budai, D. P. Norton, D. K. Christen, A. Goyal,[1] D. M. Kroeger,[1] E. D. Specht,[1]
Q. He,[2] M. Paranthaman,[3] B. Saffian,[4] F. A. List,[1] B. C. Sales, and D. Lee[1]

Applications of high-T_c superconductors (HTSc) require that key materials properties be understood and controlled. Because weak-linked grain boundaries in polycrystalline materials result in low values for the critical current density, J_c, the fabrication of crystallographically oriented wires remains a high priority. Previous work at ORNL has shown that in-plane epitaxy can be achieved for YBaCuO films grown on the surfaces of textured and single-crystal metal substrates.[5,6] This approach has now been successfully utilized in the fabrication of HTSc films on roll-textured metal substrates, yielding $J_c \sim 10^6$ A/cm^2 at 77 K.[7]

The initial metal substrate used in the ORNL approach is a biaxially textured {100}⟨001⟩ Ni tape formed by cold-rolling and recrystallization.[8] Epitaxial CeO_2 and YSZ buffer layers deposited by pulsed-laser deposition maintain the orientation of the Ni grains, while providing a chemical diffusion barrier and mechanical stability. The final HTSc c⊥ YBaCuO layer is also in-plane aligned by the substrate.

X-ray diffraction scans show that all layers of the YBaCuO/YSZ/CeO_2/Ni composite are oriented with (001) planes parallel to the surface. Furthermore, as shown in Fig. 1, the in-plane texture of all layers mimics that of the Ni substrate ($\Delta\phi \sim 6°$), while the out-of-plane texture of the YBaCuO ($\Delta\theta \sim 1°$) is reduced by the low (001) surface energy.

Based on this research, roll-textured substrates are expected to provide a rapid, low-cost technique for producing long-length, high-current superconducting wires. The ORNL approach has been licensed by two companies.

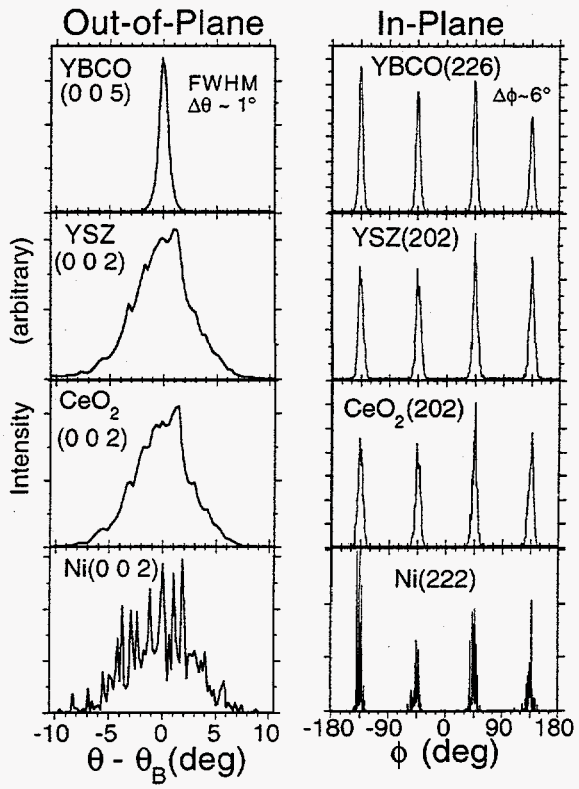

Fig. 1. X-ray scans showing alignment of a YBCO/YSZ/CeO_2 film on roll-textured Ni.

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1. Metals and Ceramics Division, ORNL.
2. Graduate student from The University of Tennessee.
3. Chemistry Division, ORNL.
4. Graduate student from the University of Tennessee. Present Address: Oxford Instruments, Cambridge, U.K.

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6. J. D. Budai et al., *SSD Progress Reports:* Sept. 1993, p. 193, 195; March 1995, p. 192.
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CONTROLLING SEMICONDUCTOR NANOCRYSTALS USING METASTABLE PHASE RECRYSTALLIZATION[1]

J. D. Budai, C. W. White, S. P. Withrow, M. F. Chisholm, J. G. Zhu,[2] and R. A. Zuhr

The fabrication and use of semiconductor nanocrystals with size-dependent electro-optical properties are areas of intensely active research because of their potential applications which include quantum-dot lasers, high-speed nonlinear optical switches, and single-electron transistors. A new approach for controlling the size, orientation, and lattice structure of semiconductor nanocrystals is being used. This approach exploits ion-induced amorphization and epitaxial substrate recrystallization to control microstructural changes in nanocrystals formed in single-crystal alumina. The underlying physical mechanisms involve changes in impurity solubility, crystal symmetry, and cation bonding of the substrate.

In the ion implantation approach for synthesizing semiconductor nanocrystals, ions are injected into the surface region of the substrate, and quantum dots are formed by precipitation from the supersaturated solid solution during subsequent thermal annealing. In this study, implantation was carried out in two distinct regimes. In the low ion-damage regime, the substrate remained in the α-Al_2O_3 phase, and the nanocrystal microstructure was controlled by the properties of the sapphire substrate. In high-damage cases, the substrate was amorphized during implantation and subsequently recrystallized during annealing in the form of metastable γ-Al_2O_3. Semiconductor nanocrystals precipitated within this matrix exhibited significant changes in their precipitation kinetics, their orientation, and even their lattice structure. For example, as shown in Fig. 1, hexagonal CdSe was formed in α-Al_2O_3, while cubic CdSe was formed in γ-Al_2O_3.

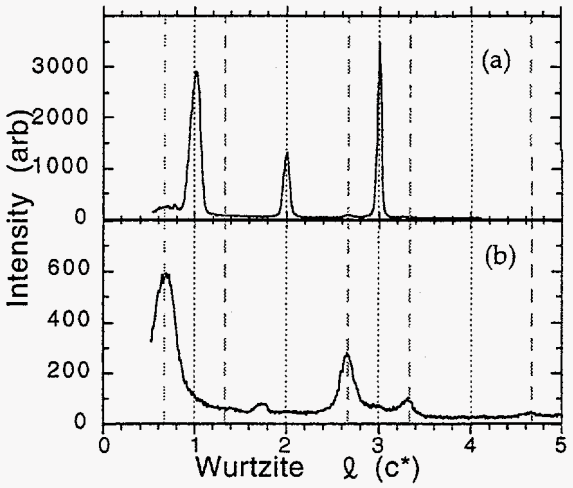

Fig. 1. X-ray ℓ-scans from CdSe nanocrystals precipitated in (a) α–Al_2O_3 and (b) γ-Al_2O_3.

The observed structural differences can be explained by considering the related, but distinct, lattice structure of the α-(rhombohedral) and γ-(cubic) alumina matrices. Furthermore, these concepts can be extended beyond semiconductor nanocrystals to essentially any precipitate, as well as to epitaxial thin films. The ability to control the microstructure of nanocrystals provides exciting opportunities both in basic investigations of physical properties of nanocrystals and in applications utilizing nanostructured materials.

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1. Summary of paper: *Nature* (in press).
2. ORNL/ORISE postdoctoral research associate. Present address: New Mexico State University, Las Cruces, N. Mex.

UNI–CAT BEAM LINE PROGRESS AT THE ADVANCED PHOTON SOURCE

B. C. Larson, G. E. Ice,[1] J. Z. Tischler, P. Zschack,[2] J. D. Budai, E. D. Specht,[1] and D. H. Lowndes

The Oak Ridge National Laboratory (ORNL), University of Illinois (UIUC), National Institute of Standards and Technology (NIST), and UOP, Inc., collaborative beam line at the Advanced Photon Source (APS) brought its first monochromatic beam into the experimental hutch in May 1997. The undulator x-ray beam of the University, National Laboratory, Industry–Collaborative Access Team (UNI–CAT) project obtained a 28-keV x-ray beam with a fluence of 1×10^{12} photons per s in an area 0.3-mm width by 0.5-mm height. This represents a factor of 5 better horizontal focusing and a factor of 2 better vertical focusing than the ORNL-UIUC X-14 beam line at the National Synchrotron Light Source at Brookhaven National Laboratory. It also represents an increase of 2–3 orders of magnitude in fluence for this energy.

A vertical focusing x-ray mirror system and a high-resolution eight-circle diffractometer are under procurement for delivery in December 1997, and monochromatic beam conditioning components, including capabilities for high-resolution secondary monochromators, beam conditioning mirrors, and x-ray microscope stages (constructed at NIST), are undergoing tests. Initial scientific experiments on the undulator beam line are anticipated in October 1997. An excimer laser-ablation film deposition system (designed in collaboration with UIUC) is scheduled for delivery in October 1997 to be used in connection with fundamental nonequilibrium film-growth investigations and superhard material deposition studies.

The final design report for the bend-magnet beam line for UNI–CAT is near completion, with construction to begin upon approval. The bend magnet beam line will have both sagittal and vertical focusing and will feature interchangeable Si ⟨111⟩ and ⟨110⟩ monochromator crystals for high-resolution extended x-ray absorption spectroscopy. A second experimental hutch will accommodate high-resolution x-ray topography and microscopy, small-angle scattering, diffuse scattering, and general diffraction physics.

In addition, the APS Proposal Evaluation Board has approved the addition of Sector 34 to the UNI–CAT project for the development of a microbeam diffraction facility (UNI–CAT-II). Kirkpatrick-Baez mirrors and phase zone-plate lenses will provide for submicron resolution white and monochromatic microbeam x-ray diffraction and coherent scattering. This dedicated microbeam facility will be a collaborative effort between ORNL and UIUC with funding from the National Science Foundation as well as the Department of Energy Basic Energy Sciences.

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1. Metals and Ceramics Division, ORNL.
2. UNI-CAT–University of Illinois, Urbana, Ill.

VARIATION OF q WITH ENERGY IN LOSS SPECTRA MEASURED USING MOSAIC ANALYZERS[1]

J. Z. Tischler, B. C. Larson, and P. Zschack[2]

Measurements of the dynamical structure factor, $S(q,\omega)$, as a function of wave vector q and energy ω, are an important method for investigating dynamical electronic properties of materials. Such measurements provide direct information on many-body effects and electron correlations needed to obtain a detailed understanding of materials.

Inelastic x-ray scattering measurements of $S(q,\omega)$ require moderate q resolution and an energy resolution of a few electron volts or less. Unfortunately, even using second- and third-generation synchrotron sources, inelastic scattering intensities are very low. As a result, considerable effort has been expended in designing detector/analyzer systems that collect the scattering over large solid angles with good energy resolution.

Most inelastic x-ray scattering measurements are performed using thin, spherically bent Si (or Ge) crystal analyzers, which collect X rays over a sizable range in q, at a single energy. An alternative approach utilizes a cylindrically bent graphite mosaic analyzer in which the inelastically scattered X rays are focused onto a linear detector, providing the entire energy loss spectrum simultaneously.[3]

Because the mosaic spread of pyrolytic graphite analyzers (~0.5°) is normally much smaller than the angle subtended by the analyzer (~4°), the q resolution is sharp, but the wave vector changes with energy. Although this wave vector change has been ignored generally, it has been found that the shift in q is not negligible. The shift with energy is shown in Fig. 1 for wave vectors typical for x-ray measurements of $S(q,\omega)$. Clearly, the size of the variation is sufficiently large that it must be considered in inelastic scattering analyses.

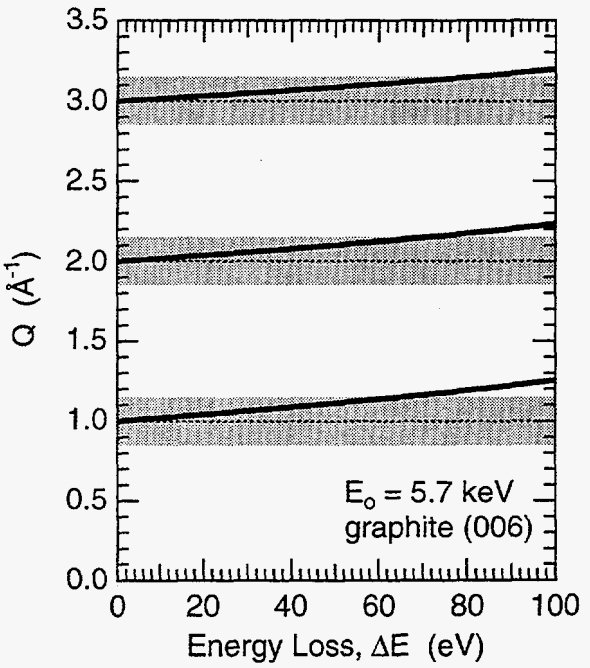

Fig. 1. The actual q for a mosaic analyzer at three different wave vectors for a 100-eV loss spectrum and 5.7-keV incident X rays. The gray bands show a typical q resolution for a spherically bent perfect crystal analyzer. The q resolution for a mosaic analyzer is approximately the thickness of the solid line.

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2. University of Illinois, Urbana, Illinois. Present address: UNICAT, Argonne National Laboratory, Argonne, Ill.
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Third International Conference on Laser Ablation (COLA '95), Strasbourg, France, May 22–26, 1995:

D. B. Geohegan and A. A. Puretzky, "Laser Ablation Plume Thermalization Dynamics in Background Gases: Combined Imaging, Optical Absorption and Emission Spectroscopy, and Ion Probe Measurements"

J. N. Leboeuf, K. R. Chen, J. M. Donato, D. B. Geohegan, C. L. Liu, A. A. Puretzky, and R. F. Wood, "Dynamical Modeling of Laser Ablation Processes" (invited paper)

C.-L. Liu, J. N. Leboeuf, R. F. Wood, D. B. Geohegan, A. A. Puretzky, J. M. Donato, and K. R. Chen, "On the Mechanisms of 'Plume Splitting' and Vapor Breakdown"

C.-L. Liu, J. N. Leboeuf, R. F. Wood, D. B. Geohegan, A. A. Puretzky, J. M. Donato, and K. R. Chen, "Numerical Simulation Studies of Pulse Scattering Mechanisms During Laser Ablation into Background Gases" (invited paper)

D. P. Norton, B. C. Chakoumakos, and J. D. Budai, "Formation of Artificially Layered High-Temperature Superconductors Using Pulsed-Laser Deposition" (invited paper)

A. A. Puretzky, D. B. Geohegan, G. E. Jellison, Jr., and M. M. McGibbon, "Comparative Diagnostics of ArF- and KrF-Laser Generated Carbon Plumes Used for Amorphous Diamond-Like Carbon Film Deposition" (invited paper)

International Workshop on Condensed Matter Theory, Caracus, Venezuela, June 18–22, 1995:

J. J. Quinn, "Composite Fermion Excitations in Fractional Quantum Hall Systems" (invited paper)

International Workshop on Two-Dimensional Electronic Systems, Ottawa, Canada, June 1995:

J. J. Quinn, "Fermi Liquid Shell Model and the Energy Spectra of Quantum Hall Systems" (invited paper)

Fourth International Conference on Trends in Welding Research, Gatlinburg, Tennessee, June 5–9, 1995:

L. A. Boatner, J. B. Sipf, M. Rappaz, D. Corrigan, and S. A. David, "Surface Morphological Properties of Stationary GTA and E-Beam Melt Pools"

J. B. Sipf, L. A. Boatner, and S. A. David, "Solidification Microstructures in Single-Crystal Stainless Steel Melt Pools"

S. Spooner, S. A. David, X. L. Wang, C. R. Hubbard, J. H. Root, I. Swainson, and T. M. Holden, "Residual Stresses in Austenitic Steel Weldments: Measurements of Lattice Parameter and Ferrite Constitution Using Neutron Diffraction"

S. Spooner, "Role of Phase Transformations in Residual Stress Development in Multipass Ferritic Steel Welds and Gleeble Test Bars"

S. Spooner, S. A. David, and C. R. Hubbard, "Role of Phase Transformations in Residual Stress Development in Multipass Ferritic Steel Welds and Gleeble Test Bars"

The Royal Society Discussion Meeting on Three Dimensional Chemical Characterization of Electronic Materials," London, United Kingdom, June 7–8, 1995:

S. J. Pennycook, N. D. Browning, M. M. McGibbon, A. J. McGibbon, D. E. Jesson, and M. F. Chisholm, "Atomic-Scale Imaging and Analysis with the Scanning Transmission Electron Microscope" (invited paper)

The 9th International Summer School on Crystal Growth, Arnhem, the Netherlands, June 11–16, 1995:

L. A. Boatner, H.-M. Christen, and J. O. Ramey, "Impurity Segregation Effects in the Growth of Pure and Mixed Tantalate/Niobates in Semiconducting and Insulating Forms"

CAM 95 Physics Meeting, CAP Congress 1995, Quebec, Canada, June 11–16, 1995:

H. A. Mook, "Recent Results on High-Temperature Superconductors" (invited paper)

55th Annual Conference on Physical Electronics, Flagstaff, Arizona, June 12–14, 1995:

H. Graupner and D. M. Zehner, "Composition and Structure of FeAl Low-Index Surfaces"

A. Hanbicki, "Hydrogen on NiAl(110)"

1995 International Workshop on Superconductivity, Maui, Hawaii, June 18–21, 1995:

D. K. Christen, Q. He, M. Paranthaman, C. E. Klabunde, R. Feenstra, A. Goyal, F. A. List, D. M. Kroeger, J. E. Tkaczyk, J. A. Deluca, Z. R. Ren, C. A. Wang, and J. H. Wang, "Superconducting Transport Properties of T1-1223 Deposits on Polycrystalline Substrates"

R. Feenstra, D. P. Norton, J. D. Budai, E. C. Jones, D. K. Christen, and T. Kawai, "Defect Formation and Carrier Doping in Epitaxial Films of the 'Parent' Compound $SrCuO_2$: Synthesis of Two Superconducting Descendants" (invited paper)

The 11th International Conference on Crystal Growth, The Hague, the Netherlands, June 18–23, 1995:

L. A. Boatner, H.-M. Christen, and J. O. Ramey, "Impurity Segregation Effects in the Growth of Pure and Mixed Tantalate/Niobates in Semiconducting and Insulating Forms"

International Conference on Surface Science: Critical Review and Outlook, Hong Kong, June 19–23, 1995:

Z. Zhang, "Atomic-Scale Manipulation of Growth Kinetics and 2D Island Shapes" (invited paper)

Conference on Amphiphilic Molecules, Micellar Structures, and Mesophases, Jülich, Germany, June 23–24, 1995:

L. J. Magid, J. B. Hayter, P. D. Butler, and W. A. Hamilton, "Shear-Induced Ordering of Rodlike Micelles Near a Solid Surface" (invited paper)

International Workshop on Vortex Dynamics, Chicago, Illinois, June 24–29, 1995:

J. R. Thompson, Y. C. Kim, D. K. Christen, Y. R. Sun, M. Paranthaman, and E. D. Specht, "Surface Barriers, Irreversibility Line, and Pancake Vortices in Aligned $HgBa_2Ca_2Cu_3O_{8+\delta}$" (invited paper)

Fourth International Conference on Surface X-Ray and Neutron Scattering, Lake Geneva, Wisconsin, June 26–30, 1995:

A. P. Baddorf, "X-Ray Study of an Incommensurate Reconstruction of the FeAl(110) Surface"

A. P. Baddorf and S. S. Chandavarkar, "Identification of an Incommensurate $FeAl_2$ Overlayer on FeAl(110) Using X-Ray Diffraction and Reflectivity"

E. E. Fullerton, S. Adenwalla, G. P. Felcher, K. T. Riggs, C. H. Sowers, S. D. Baker, and J. L. Robertson, "Neutron Diffraction and Reflectivity Studies of the Cr Néel Transition in Fe/Cr(001) Superlattices"

Surface X-Ray and Neutron Scattering, Argonne, Illinois, June 25–30, 1995:

W. A. Hamilton, P. D. Butler, J. B. Hayter, L. J. Magid, and P. J. Kreke, "Over the Horizon SANS: Measurements on Near-Surface Poiseuille Shear-Induced Ordering of Dilute Solutions on Threadlike Micelles"

W. A. Hamilton, P. D. Butler, J. B. Hayter, L. J. Magid, and P. J. Kreke, "Over the Horizon SANS: Measurements on Near-Surface Shear-Induced Hexagonal Ordering of a Dilute Solution of Threadlike Micelles"

International Workshop on Semiconductor Microstructures, Glasgow, Scotland, July 1995:

J. J. Quinn, "Numerical Studies of Quantum Hall Systems" (invited paper)

First International SPIE Conference on Time-Resolved Electron and X-Ray Diffraction, San Diego, California, July 9–14, 1995:

B. C. Larson, "Time-Resolved Materials Science Opportunities Using Synchrotron X-Ray Sources" (invited paper)

Sixteenth International Conference on Atomic Collisions in Solids (ICACS-16), Linz, Austria, July 17–21, 1995:

M. T. Robinson, "Binding Energy Effects in Cascade Evolution and Sputtering"

International Cryogenic Materials Conference (ICMC-95), Columbus, Ohio, July 17–21, 1995:

J. G. Ossandon, J. R. Thompson, Y. R. Sun, Y, C. Kim, D. K. Christen, and B. C. Chakoumakos, "Increases of H_{c2} in BiPb-2223 by Radiation-Induced Defects"

X-Rays and the Electronic Structure of Solids; International Symposium on the Occasion of the 100th Anniversary of the Discovery of X Rays, Würzburg, Germany, July 20–21, 1995:

A. G. Eguiluz, "Many-Electron and Band-Structure Effects in the Collective Excitations of Metals" (invited paper)

Eighth International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques, Snowmass Village, Colorado, July 23–28, 1995:

M. A. George, K.-T. Chen, A. Burger, D. Nason, and L. A. Boatner, "Heavy Metal Iodides Examined by Atomic Force Microscopy" (invited paper)

American Crystallographic Association Annual Meeting, Montreal, Quebec, Canada, July 23–28, 1995:

B. C. Chakoumakos and C.-K. Loong, "Brucite $Mg(OD)_2$ Hydrogen Bonding Structure and Dynamics"

Q. Huang, B. C. Chakoumakos, J. W. Lynn, A. Santoro, R. J. Cava, J. J. Krajewski, and W. F. Peck, "Neutron Powder Diffraction Study of the Structures of $HoNi_{1.985}Co_{0.015}B_2C$, HoNiBC, and $La_3Ni_2B_2N_{3-x}$"

J. L. Robertson, C. J. Sparks, G. E. Ice, and X. Jiang, "Local Atomic Arrangements in Chemically Disordered Crystals Studied by Anomalous X-Ray Scattering" (invited paper)

Fourty-Fourth Annual Denver X-Ray Conference, Colorado Springs, Colorado, July 31–August 3, 1995:

S. Spooner and E. B. S. Purdue, "Neutron and X-Ray Scattering Studies of the Metallurgical Condition and Residual Stresses in Weldalite Welds"

13th University Conference on Glass Science, Rensselaer Polytechnic Institute, Troy, New York, August 9–11, 1995:

T. S. Anderson, R. H. Magruder, III, and R. A. Zuhr, "Effects of Substrate Temperature on the Microstructure and Optical Properties of Indium-Implanted High-Purity Silica"

53rd Annual Meeting of the Microscopy Society of America, Kansas City, Missouri, August 13–17, 1995:

W. Jiang, M. G. Norton, and D. B. Poker, "Surface Morphology of Xenon-Implanted Single-Crystal Magnesium Oxide Observed by Atomic Force Microscopy"

S. J. Pennycook, D. E. Jesson, and D. R. Liu, "Z-Contrast Imaging of Catalysts in the 300-kV STEM" (invited paper)

1995 Meeting of the IRIS Specialty Group on Infrared Materials, Ann Arbor, Michigan, August 15, 1995:

S. W. Allison, L. A. Boatner, and B. C. Sales, "High-Index, Radiation-Resistant Phosphate Glass"

American Ceramic Society Meeting, Chicago, Illinois, August 20–24, 1995:

P. D. Butler, J. B. Hayter, W. A. Hamilton, and L. J. Magid, "Use of Complementary Neutron Techniques in Studying the Effect of a Solid/Liquid Interface on Bulk Solution Structures" (invited paper)

International Conference on Superlattices, Microstructures, and Microdevices, Cincinnati, Ohio, August 21–25, 1995:

D. P. Norton, B. C. Chakoumakos, and J. D. Budai, "Formation of Artificially Layered High-Temperature Superconductors Using Pulsed-Laser Deposition" (invited paper)

International Conference on Advanced Materials (IV-ICAM'95), Cancun, Mexico, August 27–September 1, 1995:

J. D. Budai, C. W. White, S. P. Withrow, and J. G. Zhu, "Synthesis, Physical Properties, and Orientation Control of Nanocrystals Formed by Ion Implantation"

C. W. White, J. D. Budai, J. G. Zhu, S. P. Withrow, D. O. Hembree, Jr., R. A. Zuhr, D. O. Henderson, and R. H. Magruder, III, "Compound Semiconductor Nanocystals Formed by Sequential Ion Implantation"

S. P. Withrow, C. W. White, J. D. Budai, J. G. Zhu, D. M. Hembree, Jr., and C. T. Olmstead, "Characterization of Si Nanocrystals Formed by Ion Implantation into SiO_2"

J. G. Zhu, C. W. White, R. Mu, A. Ueda, D. O. Henderson, Y. Chen, S. P. Withrow, and J. D. Budai, "Photoluminescence of Ge Nanocrystals in SiO_2 on Si Substrates"

Gettering and Defect Engineering in Semiconductor Technology, Wulkow/Neuhardenberg, Germany, September 2–7, 1995:

S. J. Pennycook, N. D. Browning, M. M. McGibbon, A. J. McGibbon, M. F. Chisholm, and D. E. Jesson, "Determination of Interface Structure and Bonding by Z-Contrast STEM" (invited paper)

The Second European Congress on Catalysis, Maastricht, the Netherlands, September 3–8, 1995:

A. T. Hanbicki, E. W. Plummer, A. P. Baddorf, B. Hammer, and M. Scheffler, "An Experimental-Theoretical Investigation of the Interaction of Hydrogen with a NiAl Surface"

9th International Conference on Surface Modification of Metals by Ion Beams, San Sebastian, Spain, September 4–8, 1995:

J. M. Williams and L. Riester, "Properties of Nitrogen-Ion-Implanted and Comparison Materials"

15th European Conference on Surface Science, Lille, France, September 4–8, 1995:

M. Okada, A. P. Baddorf, and D. M. Zehner, "Adsorption of Hydrogen on $Mo_{1-x}Re_x$(110) Surfaces"

K. Pohl, J. B. Hannon, D. B. Poker, and E. W. Plummer, "Structural Study of the H/Be(0001) Surface"

HEPAP Composite Subpanel for the Assessment of the Status of Accelerator Physics and Technology, Chicago, Illinois, September 8–10, 1995:

J. B. Roberto, "Use of Accelerators in Surface Modification R&D" (invited paper)

The First Polish-U.S. Conference on High-Temperature Superconductivity, Wroclaw, Poland, September 11–15, 1995:

D. C. Johnston, T. Ami, F. Borsa, P. C. Canfield, P. Carretta, B. K. Cho, J. H. Cho, F. C. Chou, M. Corti, M. K. Crawford, P. Dervenagas, R. W. Erwin, J. A. Fernandez-Baca, A. I. Goldman, R. J. Gooding, Q. Huang, M. F. Hundley, R. L. Harlow, B. N. Harmon, A. Lascialfari, L. L. Miller, J. E. Ostenson, N. M. Salem, C. Stassis, B. Sternlieb, B. J. Suh, D. R. Torgenson, D. Vaknin, K. J. E. Vos, X.-L. Wang, Z. R. Wang, M. Xu, and J. Zarestky," Overview of Recent Magnetic Studies of High-T_c Cuprate Parent Compounds and Related Materials" (invited paper)

J. R. Thompson, "The Impact of Tailored Defects on Length Scales and Current Conduction in High-T_c Superconductors" (invited paper)

Electron Microscopy and Analysis Group Conference (EMAG 95), Birmingham, United Kingdom, September 12–15, 1995:

S. J. Pennycook, D. E. Jesson, M. M. McGibbon, A. J. McGibbon, P. D. Nellist, and N. D. Browning, "Microanalysis at the Atomic Level" (invited paper)

North American Conference on Molecular Beam Epitaxy, College Park, Maryland, September 17–20, 1995:

K. M. Chen, D. E. Jesson, S. J. Pennycook, T. Thundat, and R. J. Warmack, "New Insights into the Kinetics of the Stress-Driven 2D-to-3D Transition"

Gordon Research Conference on Superconductivity, Les Diablerets, Switzerland, September 17–22, 1995:

D. P. Norton, "Synthesis of Artificially Layered Cuprate Superconductors by Pulsed-Laser Deposition" (invited paper)

6th International Conference on Silicon Carbide and Related Materials–1995, Kyoto, Japan, September 18–21, 1995:

R. F. Davis, S. Tanaka, R. S. Kern, J. Xu, and J. F. Wendelken, "The Initial Stages of Growth of SiC and AIN Thin Films on Vicinal and On-Axis Surfaces of 6H-SiC(0001)"

D. C. Lubben, G. E. Jellison, Jr., and F. A. Modine, "Molecular-Jet Chemical Vapor Deposition of SiC"

M. V. Rao, J. A. Gardner, O. W. Holland, G. Kelner, M. Ghezzo, D. S. Simons, and P. H. Chi, "Al and N Ion Implantations in 6H-SiC"

Eighth International Workshop on Glasses and Ceramics from Gels, Fargo, Portugal, September 18–22, 1995:

M. T. Harris, A. Singhal, J. S. Lin, and L. M. Toth, "FTIR Spectroscopy, SAXS, and Electrical Conductivity Studies of the Hydrolysis and Condensation of Zirconium and Titanium Alkoxides"

Second Workshop on Software Development at Neutron Scattering Sources (SoftNeSS'95), Gaithersburg, Maryland, September 21–22, 1995:

J. Z. Tischler, "HDF as a Data Standard, Tutorial on HDF" (invited paper)

Dynamical Quantum Processes on Solid Surfaces, Osaka, Japan, September 20–22, 1995:

M. Okada and D. M. Zehner, "Investigation of the Effects of Hydrogen on the Dynamics of $Mo_{1-x}Re_x(110)$ Surfaces"

M. Okada, A. P. Baddorf, D. M. Zehner, and E. W. Plummer, "Effects of Hydrogen on the Dynamics of the $Mo_{0.95}/Re_{0.05}(111)$ Surface"

13th International Vacuum Congress/9th International Conference on Solid Surfaces, Yokohama, Japan, September 25–29, 1995:

G. Lee and E. W. Plummer, "Comparison of the Interaction of Hydrogen with Cu(111) and Ag(111) Surfaces"

G. Lee, D. B. Poker, D. M. Zehner, and E. W. Plummer, "Coverage and Structure of Deuterium on Cu(111)"

M. Okada and D. M. Zehner, "Hydrogen Adsorption on $Mo_{1-x}Re_x(110)$ Surfaces"

Alabama Materials Research Conference, Birmingham, Alabama, September 26–27, 1995:

A. L. Evelyn, D. Ila, J. Fisher, and D. B. Poker, "Ion Beam Modification of PVDC and PE Polymers"

D. Ila, C. C. Smith, D. B. Poker, C. Lawson, and D. Gale, "Post-Bombardment Enhanced Optical Absorption in Ion-Implanted Silica"

Y. Qian, D. Ila, K. X. He, M. Curley, and D. B. Poker, "Ion-Beam-Induced Changes in the Optical Properties of MgO"

T. Taylor, D. Ila, R. L. Zimmerman, P. R. Ashley, and D. B. Poker, "Fabrication of Optical Channel Waveguides in the GaAs/AlGaAs System by MeV Ion Beam Bombardment"

G. Terry, D. Ila, and D. B. Poker, "Electrochemical Measurements of Lithium-Ion-Bombarded Polymeric Carbon"

E. K. Williams, D. Ila, S. Sarkisov, P. Venkateswarlu, and D. B. Poker, "Ion Beam and Optical Characterization of Multilayer Waveguides in Lithium Niobate"

E. K. Williams, D. Ila, S. Sarkisov, P. Venkateswarlu, D. B. Poker, and P. R. Ashley, "Loss Measurements of Stoichiometric Ti- and O-Implanted $LiNbO_3$ Channel Waveguides"

Horizons in Small-Angle Scattering from Mesoscopic Systems, Stromboli, Italy, September 27–30, 1995:

D. Chillura-Martino, R. Triolo, J. B. McClain, J. R. Combes, D. E. Betts, D. A. Canelas, J. M. DeSimone, E. T. Samulski, H. D. Cochran, J. D. Londono, and G. D. Wignall, "Neutron Scattering Characterization of Homopolymers and Graft-Copolymer Micelles in Supercritical Carbon Dioxide" (invited paper)

A. W. Overhauser 70th Birthday Symposium, West Lafayette, Indiana, October 21, 1995:

J. J. Quinn, "Composite Fermions in Quantum Hall Systems" (invited paper)

1995 Fall Meeting of the Ceramic Society of Japan, Kyoto, Japan, October 3–5, 1995:

Y. Shigesato, I. Yasui, and T. E. Haynes, "Study of the Ion Implantation for Valence Electron and Microstructure Controls on ITO Films"

International Battery Association Chicago Meeting, Rosemont, Illinois, October 7–8, 1995:

J. B. Bates, N. J. Dudney, and D. Lubben, "Thin-Film Li-$LiMn_2O_4$ Batteries" (invited paper)

Intersociety Polymer Conference, Baltimore, Maryland, October 7–10, 1995:

S. Talibuddin, J. P. Runt, and J. S. Lin, "Microstructure of Crystalline Polymer Blends"

G. D. Wignall, J. D. Londono, R. G. Alamo, and L. Mandelkern, "The Morphology of Blends of Linear and Branched Polyethylenes" (invited paper)

188th Meeting of the Electrochemical Society, Chicago, Illinois, October 8–13, 1995:

J. B. Bates, D. Lubben, N. J. Dudney, and F. X. Hart, "Five-Volt and 4.6-V Plateaus in $LiMn_2O_4$ Thin Films"

N. J. Dudney, J. B. Bates, D. Lubben, and F. X. Hart, "Thin-Film Rechargeable Lithium Batteries with Amorphous $Li_xMn_2O_4$ Cathodes"

B. S. Kwak and J. B. Bates, "Capacity Fade in Thin-Film Lithium-αV_2O_5 Cells"

B. Wang, J. B. Bates, C. F. Luck, B. C. Sales, R. A. Zuhr, and J. D. Robertson, "Sputter Deposition and Characterization of Lithium Cobalt Oxide Thin Films and Their Applications in Thin-Film Rechargeable Lithium Batteries"

X. Yu, J. B. Bates, and G. E. Jellison, Jr., "Characterization of Lithium Phosphorous Oxynitride Thin Films"

The Sixth Eastern Regional Conference on Crystal Growth, Atlantic City, New Jersey, October 15–18, 1995:

K.-T. Chen, W. E. Collins, M. A. George, J. Tong, A. Burger, D. Nason, R. B. James, E. Soria, E. Cross, and L. A. Boatner, "Bismuth-Rich Precipitates in Bismuth Tri-Iodide Crystals"

42nd National Symposium of the American Vacuum Society, Minneapolis, Minnesota, October 16–20, 1995:

A. P. Baddorf, "Experimental Evaluation of Anharmonicity at Metal Surfaces" (invited paper)

C. Doughty, S. M. Gorbatkin, D. B. Poker, R. L. Rhodes, L. A. Berry, and S. M. Rossnagel, "Liner Formation and Feature Filling in a Cu Permanent Magnet Electron Cyclotron Resonance (ECR) Plasma Deposition System"

S. M. Gorbatkin, F. C. Doughty, R. L. Rhodes, W. C. Oliver, K. B. Alexander, T. Y. Tsui, G. M. Pharr, and D. L. Medlin, "Hard Boron Suboxide Thin-Film Deposition Using Electron Cyclotron Resonance (ECR) Microwave Plasmas"

D. B. Poker, R. L. Rhoades, and B. S. Mercer, "ECR Plasma Etching of Materials for Ferroelectric Applications"

A. K. Swan and J. F. Wendelken, "Flux Dependence in the Growth Kinetics of Cu(100) Sub-Monolayer Homoepitaxy"

J. F. Wendelken, J. M. Carpinelli, J.-K. Zuo, and D. M. Zehner, "Step-Step Interactions on TaC(N10) Surfaces Studied with SPALEED and STM"

F. Wu, Z. Y. Zhang, M. Bott, and M. G. Lagally, "Microscopic Mechanism and Characteristics of Island Coarsening During the Growth and Subsequent Annealing of Si and Si(001)"

D. M. Zehner, M. Okada, A. P. Baddorf, L. Hammer, M. Kottcke, S. Meyer, C. Rath, and K. Heinz, "Structure and Composition of Clean and Hydrogen-Covered $Mo_{0.75}Re_{0.25}$ (110) Surfaces"

Seventh U.S.-Japan Workshop on High-T_c Superconductors, Tsukuba, Japan, October 24–25, 1995:

D. K. Christen, Q. He, M. Paranthaman, C. E. Klabunde, R. Feenstra, A. Goyal, F. A. List, E. D. Specht, D. M. Kroeger, J. E. Tkaczyk, J. A. DeLuca, Z. F. Ren, C. A. Wang, and J. H. Wang, "Transport Properties of Tl1223 Deposits for Possible Conductor Applications" (invited paper)

23rd International Thermal Conductivity Conference, Nashville, Tennessee, October 29–November 1, 1995:

P. Hyldgaard and G. D. Mahan, "Phonon Knudsen Flow in GaAs/AlAs Superlattices"

International Symposium on the Science and Technology of Atomically Engineered Materials, Richmond, Virginia, October 30–November 4, 1995:

R. F. Haglund, Jr., D. H. Osborne, R. H. Magruder, III, C. W. White, R. A. Zuhr, D. E. Hole, P. D. Townsend, F. Gonella, and P. Mazzoldi, "Metal Quantum-Dot Composites as Nonlinear Waveguide Materials" (invited paper)

F. Liu, M. Mostoller, T. Kaplan, S. N. Khanna, and P. Jena, "Evidence for a New Class of Solids: First-Principles Study of $K(Al_{13})$" (invited paper)

Forth-Seventh Pacific Coast Regional Meeting of the American Ceramic Society, Seattle, Washington, November 1–3, 1995:

H. A. Mook, "Neutron Scattering from High-Temperature Superconductors" (invited paper)

The American Ceramic Society Fall Meeting, New Orleans, Louisiana, November 5–8, 1995:

L. A. Boatner, J. R. Brewster, J. D. Budai, and J. Rankin, "The Morphological Properties of Faceted Particles and the Control of Ceramic Microstructures"

B. C. Sales, S. W. Allison, L. A. Boatner, J. J. Garefino, G. E. Jellison, Jr., and L. Gea, "New High-Numerical-Aperture Optical Fibers"

40th Annual Congress on Magnetism and Magnetic Materials, Philadelphia, Pennsylvania, November 6–9, 1995:

E. E. Fullerton, K. T. Riggs, C. H. Sowers, S. D. Badger, A. Badger, and J. L. Robertson, "Interlayer Coupling Transition at the Cr Néel Temperature in Fe/Cr(001) Superlattices"

J. A. Fernandez-Baca, P. Hill, B. C. Chakoumakos, and N. Ali, "Neutron Diffraction Study of the Magnetic Structures of $CeMn_2Ge_2$ and $CeMn_2Si_2$"

Thirty-Seventh Annual Meeting of the Division of Plasma Physics, American Physical Society, Louisville, Kentucky, November 7–10, 1995:

J. N. Leboeuf, K. R. Chen, J. M. Donato, D. B. Geohegan, C. L. Liu, A. A. Puretzky, and R. F. Wood, "Dynamical Modeling of Laser Ablation Processes for Thin-Film Deposition of Materials," [*Bull. Am. Phys. Soc.* **40**, 1644 (1995)] (invited paper)

C. C. Tsai, G. C. Barber, E. H. Lee, L. K. Mansur, D. E. Schechter, W. L. Stirling, J. H. Whealton, and J. M. Williams, "Multicharged-Ion Plasma Source for Ion Implantation" [*Bull. Am. Phys. Soc.* **40**, 1685 (1995)]

2nd Annual Advanced Techniques for Replacing Chromium: An Information Exchange, Champion, Pennsylvania, November 7–8, 1995:

J. M. Williams, L. Riester, R. Pandey, and A. W. Eberhardt, "Nitrogen Ion Implantation of Alloy and Comparison of Properties with Other Materials"

1995 Annual Meeting of the North Carolina Section of the Materials Research Society, Research Triangle Park, North Carolina, November 10, 1995:

T. E. Haynes, "Late Bloomers: Emerging Applications for Ion Beams in Materials Research" (invited paper)

Southeastern Section of the American Physical Society, Tallahassee, Florida, November 11, 1995:

D. H. Lowndes, "Semiconductor Film Growth by Pulsed-Laser Ablation" (invited paper)

American Institute of Chemical Engineers Annual Meeting, Miami Beach, Florida, November 12–17, 1995:

A. Singhal, L. M. Toth, J. S. Lin, and K. Affholter, "SAXS Study on Zirconium Aqueous Solutions"

Fall Meeting of the Materials Research Society, Boston, Massachusetts, November 27–December 1, 1995:

J. D. Budai, C. W. White, S. P. Withrow, and J. G. Zhu, "Structure and Orientation of Semiconductor Nanocrystals Formed in Insulators by Ion Implantation"

K. M. Chen, D. E. Jesson, S. J. Pennycook, T. Thundat, and R. J. Warmack, "Self-Limiting Growth Kinetics of 3D Coherent Islands" (invited paper)

M. F. Chisholm, M. Mostoller, and J. F. Wendelken, "Atomic-Scale Studies of the $\Sigma = 13\{150\}\langle 001\rangle$ Tilt Grain Boundary in Silicon"

D. K. Christen, Q. He, M. Paranthaman, C. E. Klabunde, R. Feenstra, A. Goyal, F. A. List, D. M. Kroeger, J. E. Tkaczyk, J. A. Deluca, Z. F. Ren, C. A. Wang, and J. H. Wang, "Properties of Superconducting Tl1223 Deposits on Polycrystalline Substrates"

H.-M. Christen, L. A. Boatner, L. Q. English, L. A. Gea, P. J. Marrero, and D. P. Norton, "Pulsed-Laser Deposition of Epitaxial $Sr(Ru_xSn_{1-x})O_3$ Thin-Film Electrodes and $KNbO_3/Sr(Ru_xSn_{1-x})O_3$ Bilayers"

H.-M. Christen, D. P. Norton, J. D. Budai, L. A. Gea, P. J. Marrero, and L. A. Boatner, "Superlattices of Epitaxial Ferroelectric $KNbO_3$ and Paraelectric $KTaO_3$ Films"

A. L. Evelyn, D. Ila, J. Fisher, and D. B. Poker, "Ion Beam Modification of PVDC and PE Polymers"

R. Feenstra, D. P. Norton, J. D. Budai, R. A. Zuhr, D. K. Christen, and T. Kawai, "Synthesis of HTS-Oxycarbonate Epitaxial Films"

L. A. Gea, L. A. Boatner, J. D. Budai, and R. A. Zuhr, "Formation of Vanadium Oxide Compounds in Several Oxide Substrates Implanted with Vanadium and Annealed"

L. A. Gea, L. A. Boatner, J. D. Budai, and R. A. Zuhr, "Optical Switching of Coherent VO_2 Precipitates Embedded in Sapphire"

D. B. Geohegan and A. A. Puretzky, "Species-Resolved Imaging and Gated Photon Counting Spectroscopy of Laser Ablation Plume Dynamics During KrF- and ArF-Laser PLD of Amorphous Diamond Films" (invited paper)

D. O. Henderson, A. Ueda, Y.-S. Tung, R. Mu, C. W. White, R. A. Zuhr, and J. G. Zhu, "Electronic and Vibrational Spectra of InSb Nanocrystals Embedded in a Optical Grade Fused Silica"

O. W. Holland, J. D. Budai, and B. Nielsen, "New Insight into Damage-Related Phenomena in Si Implanted Under Extreme Conditions"

E. M. Hunt, J. M. Hampikian, and D. B. Poker, "Nanocrystal Formation via Yttrium Ion Implantation into Sapphire"

N. H. Hur, B. C. Chakoumakos, M. Paranthaman, J. R. Thompson, and D. K. Christen, "The Synthesis and Characterization of $(Tl_{0.8}Bi_{0.2})(Sr_{1.6}Ba_{0.4})Ca_2Cu_3O_{9-\delta}$ Superconductor"

D. Ila, C. C. Smith, D. B. Poker, C. Lawson, and D. Gale, "Post-Bombardment Enhanced Optical Absorption in Ion-Implanted Silica"

T. Isobe, R. A. Weeks, and R. A. Zuhr, "Optical and Magnetic Properties of Silica Implanted with N^+ and Fe^+"

Y. Kim, A. Erbil, L. A. Boatner, L. Steingart, T. Mensah, and S. Hiamang, "Optical Properties of Epitaxial PLT Thin Films"

D. H. Lowndes, C. M. Rouleau, A. J. Pedraza, J. W. Park, J. D. Budai, and D. B. Poker, "Pulsed-Laser Ablation Growth and Doping of Epitaxial Compound Semiconductor Films" (invited paper)

R. Mu, A. Ueda, Y.-S. Tung, D. O. Henderson, J. G. Zhu, J. D. Budai, and C. W. White, "Stark Effects on Band Gap and Surface Phonons of Semiconductor Quantum Dots in Dielectric Hosts"

D. P. Norton, J. D. Budai, B. C. Chakoumakos, D. B. Geohegan, and A. A. Puretzky, "Epitaxial Growth of Metal Fluoride Thin Films Using Pulsed-Laser Deposition"

A. J. Pedraza, S. Cao, D. H. Lowndes, and L. F. Allard, "Laser Encapsulation of Metallic Films in SiO_2"

A. J. Pedraza, J. W. Park, D. H. Lowndes, S. Cao, and W. R. Allen, "On the Origin of Laser-Induced Surface Activation of Ceramics"

S. J. Pennycook, N. D. Browning, and M. F. Chisholm, "The Atomic Origins of the Critical Current Behavior of Grain Boundaries in $YBa_2Cu_3O_{7-\delta}$ Thin Films"

S. T. Picraux, E. Chason, J. M. Poate, J. O. Borland, M. I. Current, T. Diaz de la Rubia, D. J. Eaglesham, O. W. Holland, M. E. Law, C. W. Magee, J. W. Mayer, J. Melngailis, and A. F. Tasch, "Energetic Ion Beams in Semiconductor Processing: Summary of a DOE Panel Study"

D. B. Poker, "Solid-Phase Epitaxy of Ion-Implanted Optical Materials" (invited paper)

Y. Qian, D. Ila, K. X. He, M. Curley, D. B. Poker, and L. A. Boatner, "Ion Beam-Induced Changes in Optical Properties of MgO"

J. Rankin, L. A. Gea, and L. A. Boatner, "Annealing Studies of Ion-Implanted $KTaO_3$"

C. M. Rouleau, D. H. Lowndes, M. Strauss, S. Cao, A. J. Pedraza, D. B. Geohegan, A. A. Puretzky, and L. F. Allard, "Effect of Ambient Gas Pressure on Pulsed-Laser Ablation Plume Dynamics and ZnTe Film Growth"

T. Taylor, D. Ila, R. L. Zimmerman, P. R. Ashley, and D. B. Poker, "MeV Ion Beam Induced Index of Refraction Changes in Layered GaAs/AlGaAs Waveguides"

G. Terry, D. Ila, and D. B. Poker, "Electrochemical Measurements of Lithium Ion-Bombarded Polymeric Carbon"

J. Z. Tischler, J. D. Budai, and M. F. Chisholm, "Structure of the Ordered Atomic Interface of $CoSi_2$/Si(001) Layer by Anomalous X-Ray Scattering and Z-Contrast Imaging"

Y.-S. Tung, A. Ueda, D. O. Henderson, R. Mu, C. W. White, R. A. Zuhr, and J. G. Zhu, "Scanning Tunneling Microscopy and Atomic Force Microscopy of Au Implanted in Highly Ordered Pyrolytic Graphite"

A. Ueda, D. O. Henderson, R. Mu, Y.-S. Tung, C. Hall, J. G. Zhu, C. W. White, and R. A. Zuhr, "Vibrational and Electronic Transition in InAs Quantum Dots Formed by Sequential Implantation of In and As in a-SiO_2"

C. Uslu, B. Park, and D. B. Poker, "Ion Beam Modification of SiC for the Synthesis of Metastable Carbon-Silicon Nitride"

C. W. White, J. D. Budai, J. G. Zhu, S. P. Withrow, D. M. Hembree, D. O. Henderson, A. Ueda, Y. S. Tung, and R. Mu, "Nanocrystals and Quantum Dots Formed by High-Dose Ion Implantation"

E. K. Williams, D. Ila, S. Sarkisov, P. Venkateswarlu, and D. B. Poker, "Ion Beam and Optical Characterization of Multilayer Waveguides in Lithium Niobate"

E. K. Williams, D. Ila, S. Sarkisov, P. Venkateswarlu, and D. B. Poker, "Loss Measurements of Stoichiometric Ti- and O-Implanted $LiNbO_3$ Waveguides"

J. G. Zhu, C. W. White, D. J. Wallis, J. D. Budai, S. P. Withrow, and D. O. Henderson, "Synthesis and Properties of GaAs Nanocrystals in SiO_2 Formed by Ion Implantation"

R. A. Zuhr, R. H. Magruder, III, and T. S. Anderson, "Optical Properties of Multicomponent Antimony-Silver Nanoclusters Formed in Silica by Sequential Ion Implantation"

1995 International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 17–22, 1995:

L. J. Magid, P. D. Butler, W. A. Hamilton, and J. B. Hayter, "Structure and Dynamics in Polymer-Like Micellar Solutions Under Shear" (invited paper)

Solid State Physics Symposium, Bombay, India, December 27–31, 1995:

R. Mittal, S. L. Chaplot, N. Choudhury, C. K. Loong, and L. A. Boatner, "Lattice Dynamics of $YbPO_4$ and $LuPO_4$"

EPSRC Workshops on the Basic Science of Laser Ablation and the Pulsed-Laser Deposition of Thin Films, Belfast, Northern Ireland, January 1996:

D. B. Geohegan and A. A. Puretzky, "Nanosecond Investigations of Laser Ablation Plume Dynamics During Pulsed-Laser Deposition"

SPIE Conference on Oxide Superconductors: Physics and Nanoengineering II, San Jose, California, January 27–February 2, 1996:

D. P. Norton, B. C. Chakoumakos, and J. D. Budai, "Formation and Properties of Novel Artificially Layered Cuprate Superconductors Using Pulsed-Laser Deposition" (invited paper)

12th Yokohama 21st Century Forum on Fullerenes and Laser Processing, Yokohama, Japan, January 28–30, 1996:

D. B. Geohegan and A. A. Puretzky, "Nanosecond Investigations of Laser Ablation Plume Dynamics in Vacuum and Background Gases: Cluster Growth and Pulsed-Laser Deposition" (invited paper)

SPIE Photonics West '96 Symposium, San Jose, California, January 29–February 2, 1996:

R. Feenstra, S. J. Pennycook, M. F. Chisholm, N. D. Browning, J. D. Budai, D. P. Norton, E. C. Jones, D. K. Christen, T. Matsumoto, and T. Kawai, "Defect Formation and Carrier Doping in Epitaxial Films of the Infinite-Layer Compound" (invited paper)

Mardigras Conference, Baton Rouge, Louisiana, February 15–17, 1996:

J. J. Quinn, "Composite Fermion Picture of the Energy Spectra of Fractional Quantum Hall Systems" (invited paper)

The Minerals, Metals, and Materials Society (TMS) Annual Meeting, Anaheim, California, February 4–8, 1996:

J. D. Budai, J. Z. Tischler, D. E. Jesson, P. Zschack, J.-M. Baribeau, and D. C. Houghton, "X-Ray Diffraction Studies of Nonequilibrium Order and Domains in Si_xGe_{1-x} Films on Miscut Si(001)"

K. M. Chen, D. E. Jesson, S. J. Pennycook, T. Thundat, and R. J. Warmack, "New Insights into the Kinetics of the Stress-Driven 2D-to-3D Transition"

Z. Zhang, "Atomistic Processes in Metal Epitaxy" (invited paper)

LSU High-Performance Computing Conference, February 15–17, 1996:

T. Kaplan, "Two-Dimensional Melting: Large-Scale Molecular Dynamics Simulations" (invited paper)

Thirty-Sixth Sanibel Symposium, St. Augustine, Florida, February 24–March 2, 1996:

A. G. Eguiluz, "Electronic Excitations in Metals: Their Interplay with Density Functional Theory, Quasiparticle Theory, and Linear Response Theory" (invited paper)

Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics, Athens, Georgia, March 4–9, 1996:

K. Chen, T. Kaplan, and M. Mostoller, "Large-Scale Molecular Dynamics Simulations of Two-Dimensional Melting" (invited paper)

Silicon-on-Insulation/PTAB, Austin, Texas, March 6–8, 1996:

O. W. Holland, "Formation of Ultrathin Buried Oxides in Si by Implantation" (invited paper)

Tenth Anniversary HTS Workshop on Physics, Materials, and Applications, Houston, Texas, March 12–16, 1996:

D. K. Christen, E. D. Specht, A. Goyal, Q. He, M. Paranthaman, C. E. Klabunde, R. Feenstra, F. A. List, D. M. Kroeger, J. E. Tkaczyk, J. A. Deluca, Z. F. Ren, C. A. Wang, and J. H. Wang, "Local Texture, Current Flow, and Superconductive Transport Properties of Tl1223 Deposits on Practical Substrates" (invited paper)

H. A. Mook, P. Dai, F. Dogan, K. Salama, G. Aeppli, and M. E. Mostoller, "Neutron Scattering Measurements on $YBa_2Cu_3O_{7-\delta}$" (invited paper)

Seventh International Conference on Advanced Nuclear Research, Takasaki, Japan, March 18–20, 1996:

C. W. White, J. D. Budai, J. G. Zhu, and S. P. Withrow, "New Directions for Ion Beam Processing of Optical Materials" (invited paper)

March Meeting of the American Physical Society, St. Louis, Missouri, March 18–22, 1996:

S. D. Bader, E. E. Fullerton, and J. L. Robertson, "Spin-Density-Wave Antiferromagnetism of Cr in Fe/Cr(001) Superlattices" [*Bull. Am. Phys. Soc.* **41**, 36 (1996)]

M. Bartkowiak, G. D. Mahan, F. A. Modine, and M. A. Alim, "Multiple-Breakdown Characteristic of ZnO Varistors" [*Bull. Am. Phys. Soc.* **41**, 307 (1996)]

J. D. Budai, C. W. White, S. P. Withrow, and J. G. Zhu, "Synthesis and Physical Properties of Semiconductor Nanocrystals Formed by Ion Implantation" [*Bull. Am. Phys. Soc.* **41**, 173 (1996)]

J. M. Carpinelli and H. H. Weitering, "Anomalous Electric Behavior of the Ag/Ge(111) Interface" [*Bull. Am. Phys. Soc.* **41**, 187 (1996)]

K. Chen, T. Kaplan, and M. Mostoller, "Large-Scale Molecular Dynamics Simulations of Melting in Two-Dimensional Lennard-Jones Systems: Observation of a Metastable Hexatic Phase" [*Bull. Am. Phys. Soc.* **41**, 668 (1996)]

K. M. Chen, D. E. Jesson, S. J. Pennycook, T. Thundat, and R. J. Warmack, "Self-Limiting Growth Kinetics of 3D Coherent Islands" [*Bull. Am. Phys. Soc.* **41**, 311 (1996)]

D. Chillura-Martino, J. B. McClain, D. Canelas, D. Betts, E. T. Samulski, J. M. DeSimone, G. D. Wignall, J. D. Londono, and R. Triolo, "Homopolymers and Micelles in Supercritical CO_2: A SANS Study" [*Bull. Am. Phys. Soc.* **41**, 545 (1996)]

M. F. Chisholm, "Structure and Properties of Dislocations and Grain Boundaries in Group-IV Semiconductors" [*Bull. Am. Phys. Soc.* **41**, 729 (1996)] (invited paper)

D. K. Christen, Q. He, M. Paranthaman, C. E. Klabunde, R. Feenstra, A. Goyal, F. A. List, E. D. Specht, D. M. Kroeger, J. E. Tkaczyk, and J. A. DeLuca, "Current Flow and Superconductive Transport Properties of Tl1223 Deposits on Practical Substrates" [*Bull. Am. Phys. Soc.* **41**, 798 (1996)]

H.-M. Christen, L. A. Boatner, J. D. Budai, M. F. Chisholm, L. A. Gea, and D. P. Norton, "$KTaO_3/KNbO_3$ Thin-Film Superlattices Compared to $KTa_{1-x}Nb_xO_3$ Solid-Solution Layers" [*Bull. Am. Phys. Soc.* **41**, 764 (1996)]

J. F. Cooke, J. A. Blackman, and J. M. Bass, "Itinerant-Electron Theory of Spin Waves in HCP Cobalt" [*Bull. Am. Phys. Soc.* **41**, 735 (1996)]

P. Dai, J. Zhang, H. A. Mook, S. H. Liou, and P. A. Dowben, "Experimental Evidence for the Dynamic Jahn-Teller Effect in $La_{0.65}Ca_{0.35}MnO_3$" [*Bull. Am. Phys. Soc.* **41**, 410 (1996)]

G. Eres, "Semiconductor Thin-Film Growth Using Supersonic Molecular Beams" [*Bull. Am. Phys. Soc.* **41**, 113 (1996)] (invited paper)

R. Feenstra, D. P. Norton, J. D. Budai, R. A. Zuhr, and D. K. Christen, "Pulsed-Laser Deposition of $Sr_2Cu_{1+x}O_y(CO_3)_{1-x}$ Infinite-Layer Oxycarbonate Films" [*Bull. Am. Phys. Soc.* **41**, 231 (1996)]

J. A. Fernandez-Baca, E. Fawcett, H. L. Alberts, V. Y. Galkin, and Y. Endoh, "Pressure Effects on the Spin-Density-Wave Antiferromagnetism in Cr-1.6% Si Alloys" [*Bull. Am. Phys. Soc.* **41**, 736 (1996)]

L. A. Gea, L. A. Boatner, J. Rankin, and J. D. Budai, "Phase Transition of Coherent VO_2 Precipitates in Sapphire" [*Bull. Am. Phys. Soc.* **41**, 800 (1996)]

L. Grigorian, S. Fang, G. Sumanasekera, A. Rao, G. D. Mahan, and P. Eklund, "CVD Growth of Se-Intercalated Graphite Thin Films" [*Bull. Am. Phys. Soc.* **41**, 196 (1996)]

W. A. Hamilton and M. Yethiraj, "Enhancement of Bragg Scattered Intensity by Surface Acoustic Waves in Lithium Niobate" [*Bull. Am. Phys. Soc.* **41**, 13 (1996)]

A. T. Hanbicki, G. Gvalani, E. W. Plummer, and D. M. Zehner, "The Interaction of Hydrogen with Au(111)" [*Bull. Am. Phys. Soc.* **41**, 243 (1996)]

P. Hyldgaard and G. D. Mahan, "Phonon Transport in Semiconductor Heterostructures" [*Bull. Am. Phys. Soc.* **41**, 474 (1996)]

T. Kaplan, F. Liu, M. Mostoller, M. F. Chisholm, and V. Milman, "A Large-Scale *Ab Initio* Study of Impurities in Si Edge Dislocations" [*Bull. Am. Phys. Soc.* **41**, 441 (1996)]

H. R. Kerchner and D. K. Christen, "AC Loss in Superconductive $Bi_2Sr_2Ca_2Cu_3O_x$/Ag Tape" [*Bull. Am. Phys. Soc.* **41**, 798 (1996)]

M. Kottcke, H. Graupner, L. Hammer, K. Heinz, and D. M. Zehner, "Segregation-Induced Subsurface Restructuring of FeAl(100)" [*Bull. Am. Phys. Soc.* **41**, 188 (1996)]

B. C. Larson, J. Z. Tischler, E. D. Isaacs, P. Zschack, A. Fleszar, and A. G. Eguiluz, "Inelastic X-Ray Scattering as a Probe of the Many-Body Local-Field Factor in Metals" [*Bull. Am. Phys. Soc.* **41**, 787 (1996)]

J. D. Londono, D. Chillura-Martino, R. Triolo, D. Betts, D. Canelas, J. B. McClain, E. T. Samulski, J. M. DeSimone, and G. D. Wignall, "SANS Study of Block Copolymer Micelles in Supercritical CO_2" [*Bull. Am. Phys. Soc.* **41**, 527 (1996)]

J. Li, J. Baker, J. J. Hernandez, J. G. Skofronick, S. A. Safron, and L. A. Boatner, "Surface Characterization of $KTaO_3$ (001) by Helium Atom Scattering" [*Bull. Am. Phys. Soc.* **41**, 230 (1996)]

G. D. Mahan, "Thermoelectrics" [*Bull. Am. Phys. Soc.* **41**, 58 (1996)] (invited paper)

A. Maiti, S. J. Pennycook, and S. T Pantelides, "Chemical Rebonding During As Segregation in Si Grain Boundaries" [*Bull. Am. Phys. Soc.* **41**, 441 (1996)]

A. Maiti, "Atomistic Theory of Carbon Nanotube Growth and Bending" [*Bull. Am. Phys. Soc.* **41**, 307 (1996)] (invited paper)

J. B. McClain, D. E. Betts, D. A. Canelas, E. T. Samulski, J. M. DeSimone, J. D. Londono, and G. D. Wignall, "Characterization of Polymers and Amphiphiles in Supercritical CO_2 using Small-Angle Neutron Scattering and Viscometry"

T. Michely, M. Hohage, M. Bott, M. Morgenstern, Z. Zhang, and G. Comsa, "Atomic Processes in Low-Temperature Growth of Pt on Pt(111)" [*Bull. Am. Phys. Soc.* **41**, 273 (1996)] (invited paper)

W. W. Pai, J. Zhang, and J. F. Wendelken, "Controlled Nanostructures Fabricated by STM-Assisted Chemical Vapor Deposition" [*Bull. Am. Phys. Soc.* **41**, 554 (1996)]

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B. C. Sales and D. G. Mandrus, "Electrical and Thermal Transport Properties of Filled Skutterudite Compounds" [*Bull. Am. Phys. Soc.* **41**, 116 (1996)]

Z.-P. Shi, J. F. Cooke, Z. Zhang, and B. M. Klein, "Structural, Magnetic, and Electronic Properties of Fe/Au Monatomic Multilayers" [*Bull. Am. Phys. Soc.* **41**, 490 (1996)]

Z.-P. Shi, A. K. Swan, J. F. Wendelken, and Z. Zhang, "The Important Role of Shear Motion in Cluster Diffusion and Expitaxial Growth on FCC (100) Surfaces" [*Bull. Am. Phys. Soc.* **41**, 388 (1996)]

A. K. Swan, Z. P. Shi, Z. Zhang, and J. F. Wendelken, "Flux-Induced Huge Jump in Critical Island Size in Cu(100) Submonolayer Homoepitaxy" [*Bull. Am. Phys. Soc.* **41**, 630 (1996)]

J. Tersoff, Y. Phang, Z. Zhang, C. Teichert, and M. G. Lagally, "Self-Assembly and Self-Organization of Nanostructures in Epitaxial Growth" [*Bull. Am. Phys. Soc.* **41**, 222 (1996)] (invited paper)

J. R. Thompson, L. Krusin-Elbaum, L. Civale, D. K. Christen, and A. D. Marwick, "Regimes of Vortex Pinning and Creep in $YBa_2Cu_3O_7$ Single Crystals with Au-Ion-Induced Columnar Defects" [*Bull. Am. Phys. Soc.* **41**, 713 (1996)]

J. Z. Tischler, J. D. Budai, M. F. Chisholm, C. W. White, T. Gog, and P. Zschack, "Structure of the Ordered $CoSi_2$/Si(001) Buried Interface by Anomalous X-Ray Scattering" [*Bull. Am. Phys. Soc.* **41**, 650 (1996)]

H. H. Weitering and J. M. Carpinelli, "Low-Temperature Reconstruction Pathway to the Si(111) $(\sqrt{3} \times \sqrt{3})R30°$" [*Bull. Am. Phys. Soc.* **41**, 187 (1996)]

G. D. Wignall, J. D. Londono, F. C. Stehling, R. G. Alamo, and L. Mandelkern, "Small-Angle Neutron Scattering Investigations of Liquid-Liquid Phase Separation in Heterogeneous Linear Low-Density Polyethylene" [*Bull. Am. Phys. Soc.* **41**, 52 (1996)]

M. Yethiraj, H. A. Mook, M. Nuttley, M. Wylie, E. M. Forgan, D. M. Paul, and R. Cubitt, "On the Temperature Dependence of the Flux-Line-Lattice Bragg Intensity in Twinned Samples of the High-T_c Superconductor $YBa_2Cu_3O_7$" [*Bull. Am. Phys. Soc.* **41**, 284 (1996)]

J. Zhang, D. Welipitiya, P. A. Dowben, P. I. Oden, T. Thundat, and R. J. Warmack, "Fabrication and Characterization of Large Arrays of Micro-Scale Magnetic Features by Photoassisted Organometallic Deposition" [*Bull. Am. Phys. Soc.* **41**, 740 (1996)]

Z. Zhang, "Morphological Manifestations and Quantitative Measurements of Surface Stress and Stress Anisotropy in Ge-on-Si(001) Near Monolayer Coverages" [*Bull. Am. Phys. Soc.* **41**, 222 (1996)] (invited paper)

Mexico-USA Workshop on Scientific Facilities for Materials Science, Argonne, Illinois, March 25–28, 1996:

J. D. Budai, "Nanocrystals Synthesized Using Ion Implantation at the ORNL Surface Modification and Characterization Facility" (invited paper)

J. A. Fernandez-Baca, "Neutron Scattering Research at the High-Flux Isotope Reactor at Oak Ridge" (invited paper)

XVth International Conference on Thermoelectrics (ICT96), Pasadena, California, March 26–29, 1996:

B. C. Sales and D. G. Mandrus, "Electrical and Thermal Transport Properties of Filled Skutterudite Compounds"

43rd Annual Spring Meeting of the Japan Society of Applied Physics, Saitama, Japan, March 26–29, 1996:

Y. Shigesato, I. Yasiu, and T. E. Haynes, "Study of Ion Implantation on ITO Films (1) (Microstructure Controls by O^+ and H^+ Implantation)

Y. Shigesato, I. Yasui, and T. E. Haynes, "Study of Ion Implantation on ITO Films (2) (Carrier Controls by In^+ Implantation)"

N. Taga, M. Maekawa, Y. Shigesato, I. Yasui, and T. E. Haynes, "Preparation of Heteroepitaxial In_2O_3 Films by Molecular Beam Epitaxy"

211th ACS National Meeting, New Orleans, Louisiana, March 26–29, 1996:

M. D. Dadmun, P. Butler, and W. A. Hamilton, "Response of Liquid Crystalline Polymers to an Applied Shear Flow: Steady State and Relaxation Behavior"

Spring Meeting of the Materials Research Society, San Francisco, California, April 8–12, 1996:

J. C. Coleman and D. B. Poker, "Fabrication of Beta Silicon Carbide Diodes Using Proton Isolation"

J. A. Gardner, M. V. Rao, Y. L. Tian, O. W. Holland, G. Kelner, J. A. Freitas, Jr., and I. Ahmad, "Microwave Annealing of Ion-Implanted 6H-SiC"

D. E. Jesson, K. M. Chen, S. J. Pennycook, T. Thundat, and R. J. Warmack, "Kinetic Pathways to Strain Relaxation in the Si-Ge System"

R. Morton, S. S. Lau, D. B. Poker, and P. K. Chu, "Group-II Acceptor and Carbon Co-Implantation in GaAs"

P. D. Nellist and S. J. Pennycook, "Unique Views of Materials: Atomic-Resolution Z-Contrast Imaging"

26th Symposium on Actinides, Szklarska Poreba, Poland, April 10–14, 1996:

K. M. Murdoch, M. Illemassene, N. M. Edelstein, R. Cavellec, M. Karbowiak, E. Simoni, S. Hubert, M. M. Abraham, and L. A. Boatner, "Laser Studies of the Cm^{3+} Ion in Crystals of $LuPO_4$ and Cs_2NaYCl_6"

Surface Science Colloquium, Åarhus, Denmark, April 12, 1996:

K. Pohl and E. W. Plummer, "Structural Study of the H/Be(0001) Surface" (invited paper)

1996 Annual Meeting of the American Ceramic Society, Indianapolis, Indiana, April 14–17, 1996:

M. A. Alim, M. Bartkowiak, and F. A. Mcdine, "Mott-Schottky Analysis of Capacitance Versus Voltage in Varistors"

M. F. Chisholm, S. J. Pennycook, P. D. Nellist, N. D. Browning, E. C. Dickey, and V. P. Dravid, "Prospects of Z-Contrast STEM for Ceramic Science" (invited paper)

C. K. Loong, B. C. Sales, and L. A. Boatner, "Atomic Dynamics of Crystalline and Glassy Lead Pyrophosphate"

International Conference on Metallurgical Coatings and Thin Films, San Diego, California, April 22–26, 1996:

G. E. Jellison, Jr., "The Calculations of Thin-Film Parameters from Spectroscopic Ellisometry Data" (invited paper)

Joint Meeting of the American Physical Society and the American Association of Physics Teachers, Indianapolis, Indiana, May 2–5, 1996:

J. N. Leboeuf, "Modeling of Laser Ablation Processes for Thin-Film Deposition of Materials," [*Bull. Am. Phys. Soc.* **41**, 891 (1996)] (invited paper)

5th Annual Collaborative Computational Project/Non-Crystalline Diffraction (CCP13/NCD) Workshop, Warrington, United Kingdom, May 7–9, 1996:

G. D. Wignall, "Advantages of Absolute Calibration in Small-Angle X-Ray and Neutron Scattering Studies of Polymers and Colloids" (invited paper)

10th Annual Workshop on Numerical Methods, Morgantown, West Virginia, May 8–10, 1996:

M. F. Chisholm, "Direct Imaging of the Atomic Structure of Grain Boundarie in Silicon: Theoretical Verification of Experimental Models" (invited paper)

G. D. Mahan, "Thermoelectrics" (invited paper)

Fifteenth Pfefferkorn Conference on Electron Imaging and Signal Processing, Silver Bay, New York, May 18–22, 1996:

P. D. Nellist and S. J. Pennycook, "Probe and Object Function Reconstruction in Incoherent STEM Imaging" (invited paper)

1996 Annual Meeting of the Materials Research Society of Japan, Makuhari, Japan, May 23–24, 1996:

T. E. Haynes, Y. Shigesato, I Yasui, N. Taga, and H. Odaka, "Ion Beam Modification of Transparent Conducting Indium-Tin-Oxide Films" (invited paper)

N. Taga, M. Maekawa, Y. Shigesato, I. Yasui, and T. E. Haynes, "Deposition of Hetero-Epitaxial In_2O_3 Thin Films by Molecular Beam Epitaxy"

Eighth Annual Electronic Structure Workshop, Minneapolis, Minnesota, June 1996:

A. Maiti, "Theory of Carbon Nanotube Growth and Bending"

Optical Society of America Conference on Lasers and Electro-Optics (CLEO 96), Anaheim, California, June 2–7, 1996:

D. B. Geohegan and A. A. Puretzky, "Dynamics of Laser Ablation for Thin-Film Growth by Pulsed-Laser Deposition" (invited paper)

Seventh International Workshop on Slow-Positron Beam Techniques for Solids and Surfaces, Unterageri, Switzerland, June 2–7, 1996:

B. Nielsen, P. Asoka-Kumar, K. G. Lynn, M. P. Petkov, O. W. Holland, A. van Veen, and L. O. Roellig, "Depth-Resolved Defects Spectroscopy"

European Materials Research Society Spring Meeting, Strasbourg, France, June 4–7, 1996:

U. V. Desnica, I. D. Desnica, M. Ivanda, and T. E. Haynes, "Morphology of the Implantation-Induced Disorder in GaAs"

E. Neufeld, S. Wang, R. Apetz, Ch. Buchal, R. Carius, C. W. White, and D. K. Thomas, "Effect of Annealing and H_2-Passivation on the Photoluminescence of Si Nanoclusters in SiO_2"

Frontiers of Electron Microscopy in Materials Science, Oak Brook, Illinois, June 4–7, 1996:

P. D. Nellist and S. J. Pennycook, "Incoherent Atomic-Resolution Structure Imaging"

Gordon Research Conference, Plymouth, New Hampshire, June 10, 1996:

C. M. Rouleau, D. H. Lowndes, M. A. Strauss, S. Cao, A. J. Pedraza, D. B. Geohegan, A. A. Puretzky, and L. F. Allard, "Effect of Ambient Gas Pressure on Pulsed-Laser Ablation Plume Dynamics and ZnTe Film Growth"

Microgravity Materials Science Conference, Huntsville, Alabana, June 10–11, 1996:

L. A. Boatner, D. Corrigan, S. A. David, M. Rappaz, G. Workman, and G. Smith, "Surface Morphological Properties of Stationary Melt Pools in Single Crystals of Stainless Steel" (invited paper)

Surface Analysis '96, American Vacuum Society Topical Conference, Ann Arbor, Michigan, June 12–14, 1996:

E. K. Williams, D. Ila, T. R. Watkins, S. Sarkisov, P. Venkateswarlu, D. K. Hensley, and D. B. Poker, "Studying Stacked Waveguide Formation in $LiNbO_3$"

Canadian Association of Physicists, Ottawa, Canada, June 16–19, 1996:

D. H. Lowndes, "Growth and Doping of Compound Semiconductor Films by Pulsed-Laser Ablation" (invited paper)

Eighth International Meeting on Lithium Batteries, Nagoya, Japan, June 16–21, 1996:

T. Takada, H. Hayakawa, E. Akiba, F. Izumi, and B. C. Chakoumakos, "Novel Synthesis Process and Structure Refinements of $Li_4Mn_5O_{12}$ for Rechargeable Lithium Batteries"

M. M. Thackeray, M. F. Mansuetto, and J. B. Bates, "Structural Stability of $LiMn_2O_4$ Electrodes for Lithium Batteries"

Physical Electronics Conference, Boston, Massachusetts, June 17–19, 1996:

W. W. Pai, J. Zhang, and J. F. Wendelken, "STM Observation of Friedel Oscillations: Cyclopentadienyl (C_5H_5) Adsorption of Ag(100)"

H. H. Weitering, X. Shi, and S. C. Erwin, "Experimental and Theoretical Band Dispersions of Si(111)3 × 1-Li: Do π-Bonded Si Chains Dimerize?"

J. Zhang and E. W. Plummer, "Comparison of the Bulk and Surface Lattice Structure and Dynamics of $La_{1-x}Ca_xMnO_3$"

XIth International Conference on Ion Implantation Technology, Austin, Texas, June 17–21, 1996:

E. Chason, S. T. Picraux, J. M. Poate, D. J. Eaglesham, J. O. Borland, M. I. Current, T. Diaz de la Rubia, O. W. Holland, M. E. Law, C. W. Magee, J. W. Mayer, J. Melngailis, and A. F. Tasch, "Energetic Ion Beams in Semiconductor Processing: A Panel Study"

C. W. White, J. D. Budai, S. P. Withrow, J. G. Zhu, S. J. Pennycook, R. H. Magruder, and D. O. Henderson, "Ion Beam Synthesis of Nanocrystals and Quantum Dots in Optical Materials" (invited paper)

J. G. Zhu, C. W. White, J. D. Budai, S. P. Withrow, and D. O. Henderson, "Effects of Ion Beam Mixing on the Formation of SiGe Nanocrystals by Ion Implantation"

Vortex Dynamics Workshop, Shoresh, Israel, June 24–27, 1996:

J. R. Thompson, L. Krusin-Elbaum, L. Civale, G. Blatter, D. K. Christen, and C. Feild, "Dynamics of Vortices Pinned by Columnar Defects in YBCO Crystals—Variable-Range Vortex Hopping" (invited paper)

38th Electronic Materials Conference, Santa Barbara, California, June 26–28, 1996:

K. M. Chen, D. E. Jesson, S. J. Pennycook, T. Thundat, and R. J. Warmack, "Self-Limiting Growth Kinetics of 3D Coherent Islands: A Route to Monosized Quantum Dot Arrays"

International Conference on Electronic Properties of Strongly Interacting Two-Dimensional Systems, Trieste, Italy, July 2–5, 1996:

J. J. Quinn, "Fermi Liquid Shell Model of Composite Fermions in Quantum Hall Systems" (invited paper)

Fifth World Congress on Superconductivity, Budapest, Hungary, July 7–11, 1996:

J. G. Ossandon and J. R. Thompson, "Stability of Supercurrents in BiSrCaCuO HTSC with Artificially Created Defects" (invited paper)

Twenty-First Rare-Earth Research Conference, Duluth, Minnesota, July 7–12, 1996:

K. M. Murdoch, M. Illemassene, N. M. Edelstein, R. Cavellec, M. Karbowiak, E. Simoni, S. Hubert, M. M. Abraham, and L. A. Boatner, "Laser Studies of the Cm^{3+} Ion in Crystals of $LuPO_4$"

J. C. Nipko, C.-K. Loong, S. Kern, M. M. Abraham, and L. A. Boatner, "Crystal Field Splitting and Anomalous Thermal Expansion in $YbVO_4$"

J. C. Nipko, C.-K. Loong, M. Loewenhaupt, W. Reichardt, M. Braden, and L. A. Boatner, "Lattice Dynamics of $LuPO_4$"

Third International Conference on Nanostructured Materials, Kona Hawaii, July 8–12, 1996:

C. W. White, J. D. Budai, J. G. Zhu, S. P. Withrow, D. O. Henderson, M. J. Aziz, and M. J. Yacaman, "Ion Beam Synthesis of Encapsulated Nanocrystals and Quantum Dots"

Thirteenth International Conference on Defects in Insulating Materials, Winston Salem, North Carolina, July 15–19, 1996:

D. O. Henderson, Y. S. Tung, R. Mu, A. Ueda, J. Chen, Z. Gu, C. W. White, J. G. Zhu, M. McKay, and O. Scott, "Gold-Implanted Calcium Fluoride Single Crystals: Optical Properties of Ion-Induced Defects and Metal Nanocrystals"

A. Trukhin and L. A. Boatner, "Electronic Structure of $ScPO_4$ Single Crystals: Optical and Photoelectric Properties"

Y. S. Tung, D. O. Henderson, J. Chen, Z. Gu, A. Ueda, R. Mu, C. W. White, J. G. Zhu, and R. A. Zuhr, "Gold Ion-Irradiated Muscovite Mica: Infrared and Optical Properties of Defects and Metal Nanocrystals"

A. Ueda, R. Mu, Y. S. Tung, D. O. Henderson, C. W. White, R. A. Zuhr, J. G. Zhu, and P. W. Wang, "Annealing Effects on the Surface Plasmon of MgO Implanted with Gold"

Tenth International Conference on Small-Angle Scattering, Sao Paulo, Brazil, July 21–25, 1996:

F. J. Medellin-Rodriguez, C. A. Avila-Orta, and J. S. Lin, "SAXS Interface Distribution Function of Nylon 6 to Characterize the Effect of Molecular Weight and Crystalline Structures"

G. D. Wignall, J. D. Londono, H. D. Cochran, J. M. DeSimone, J. McClain, and J. Combes, "Neutron Scattering Characterization of Polymerization Mechanisms in Environmentally Responsible Supercritical Carbon Dioxide"

23rd International Conference on the Physics of Semiconductors, Berlin, Germany, July 21–26, 1996:

D. E. Jesson, K. M. Chen, S. J. Pennycook, T. Thundat, and R. J. Warmack, "Exploring New Pathways to Quantum Dots" (Invited)

Gordon Research Conference on Particle-Solid Interactions, North Plymouth, New Hampshire, July 21–26, 1996:

L. A. Gea, L. A. Boatner, J. D. Budai, and R. A. Zuhr, "Smart Optical Surfaces Formed by Ion Implantation and Annealing"

Gordon Research Conference on Chemistry at Interfaces, Meridian, New Hampshire, July 21–26, 1996:

P. D. Butler, W. A. Hamilton, J. B. Hayter, L. J. Magid, P. J. Kreke, and T. M. Slawecki, "The Effect of a Quartz/Liquid Interface on Bulk Solution Structures Under Flow—A Neutron Study"

Third International Conference on Computer Simulation of Radiation Effects in Solids, Guildford, United Kingdom, July 22–26, 1996:

M. T. Robinson, "Attractive Interaction Potentials and the Binary Collision Approximation" (invited paper)

First International Conference on Synchrotron Radiation in Materials Science, Chicago, Illinois, July 29–August 2, 1996:

J. Z. Tischler, J. D. Budai, M. F. Chisholm, C. W. White, T. Gog, and P. Zschack, "X-Ray Scattering Measurements of the Ordered $CoSi_2$/Si(001) Buried Interface"

International Conference on Diffusion in Materials, Nordkirchen, Germany, August 12–16, 1996:

S. T. Pantelides, M. Ramamoorthy, A. Maiti, M. F. Chisholm, and S. J. Pennycook, "Complex Impurity Dynamics in Silicon"

SPIE's Annual Meeting on Optical Design and Materials, Denver, Colorado, August 4–9, 1996:

S. W. Allison, J. P. Cunningham, S. Rajic, L. A. Boatner, and B. C. Sales, "Single-Point Diamond Turning of Lead Indium Phosphate Glass"

Summer Topicals 1996, IEEE/LEOS Conference on Advanced Applications of Lasers in Materials and Processing, Keystone, Colorado, August 5–7, 1996:

D. B. Geohegan and A. A. Puretzky, "Dynamics of Pulsed-Laser Ablation for Thin-Film Growth" (invited paper)

D. H. Lowndes, C. M. Rouleau, D. B. Geohegan, A. A. Puretzky, M. A. Strauss, A. J. Pedraza, J. W. Park, J. D. Budai, and D. B. Poker, "Pulsed-Laser Deposition of Doped Epitaxial Compound Semiconductor Films" (invited paper)

International Union of Crystallography Neutron Scattering Satellite Meeting, Gaithersburg, Maryland, August 5–7, 1996:

B. C. Chakoumakos, T. B. Lindemer, and M. Yethiraj, "$YBa_2Cu_3O_{7-x}$ Structural Systematics for Equilibrium-Cooled Samples"

P. Dai, J. Zhang, H. A. Mook, E. W. Plummer, H. Y. Hwang, S. W. Cheong, G. Aeppli, S. H. Liou, and P. A. Dowben, "The Static and Dynamic Lattice Effects in CMR Materials" (invited paper)

J. Hoyt, B. C. Chakoumakos, and S. T. Misture, "Order-Disorder In Ternary Alloys, the Heusler Alloy $AlMnCu_2$"

S. E. Nagler, B. C. Chakoumakos, and H. M. Christen, "Magnetism and Phase Transitions of $SrRuO_3$"

X.-L. Wang, S. Spooner, C. R. Hubbard, and Z. L. Feng, "Residual Stress Distribution Due to the Deposition of a Short-Length Weld Metal"

S. Spooner and X.-L. Wang, "Calculation of Diffraction Peak Displacement in Residual Stress Samples Due to Partial Burial of the Sampling Volume"

Dynamics of Crystal Surfaces and Interfaces, Traverse City, Michigan, August 5–9, 1996:

"The Role of Anisotropic Surface Energy in the Morphological Evolution of Strained Films" (invited paper)

XXIth International Conference on Low-Temperature Physics, Prague, Czech Republic, August 8–14, 1996:

D. K. Christen, D. P. Norton, Q. He, J. D. Budai, A. Goyal, D. M. Kroeger, M. Paranthaman, B. Saffian, and E. D. Specht, "Biaxially Oriented Metallic Tape Substrates for High-Temperature Superconductors"

H. R. Kerchner, D. K. Christen, J. R. Thompson, and T. Armstrong, "Hysteretic Magnetic Moment of $YBa_2Cu_3O_{7-\delta}$: An Angular Study"

J. R. Thompson, J. G. Ossandon, D. K. Christen, M. Paranthaman, E. D. Specht, and Y. C. Kim, "Equilibrium Properties of Hg-Cuprate Superconductors with 1, 2, and 3 Cu-O Layers"

J. R. Thompson, L. Krusin-Elbaum, L. Civale, G. Blatter, D. K. Christen, and C. Feild, "Dynamics of Vortices Pinned by Columnar Defects in YBCO Crystals—Variable-Range Vortex Hopping"

XVIIth Congress and General Assembly of the International Union of Crystallography, Seattle, Washington, August 8–17, 1996:

M. Agamalian, R. Triolo, and G. D. Wignall, "ORNL Double-Crystal Ultra Small-Angle Neutron Scattering Facility" (invited paper)

B. C. Chakoumakos, "$YBa_2Cu_3O_{7-x}$ Structural Systematics for Equilibrium-Cooled Samples"

W. A. Hamilton, P. D. Butler, J. B. Hayter, L. J. Magid, and Z. Han, "Neutron Scattering Studies of Near-Surface Effects on Structures in Surfactant Systems" (invited paper)

B. C. Larson, J. Z. Tischler, E. D. Isaacs, P. Zschack, A. Fleszar, and A. G. Eguiluz, "Inelastic X-Ray Scattering Investigation of Electron Correlations in Aluminum"

Microscopy and Microanalysis '96, Minneapolis, Minnesota, August 11–15, 1996:

M. F. Chisholm and S. J. Pennycook, "Z-Contrast Imaging of Grain Boundaries in Semiconductors" (invited paper)

E. C. Dickey, V. P. Dravid, P. Nellist, D. J. Wallis, N. D. Browning, and S. J. Pennycook, "Atomic Structure Determination of $NiO\text{-}ZrO_2(CaO)$ and $Ni\text{-}ZrO_2(CaO)$ Interfaces Using Z-Contrast Imaging and EELS"

S. J. Pennycook, P. D. Nellist, N. D. Browning, P. A. Langjahr, and M. Rühle, "Quantitative Structure Determination of Interfaces Through Z-Contrast Imaging and Electron Energy Loss Spectroscopy" (invited paper)

J. G. Zhu, C. W. White, J. D. Budai, M. J. Yacaman, and G. Mondragon, "Microstructure of GaAs Nanocrystals Formed Inside Single-Crystalline Silicon"

J. G. Zhu, C. W. White, J. D. Budai, and S. P. Withrow, "TEM Study of CdS Nanocrystals Formed in SiO_2 by Ion Implantation"

Gordon Conference on Point and Line Defects in Semiconductors, Andover, Massachusetts, August 18–23, 1996:

O. W. Holland, "Ion Beam Synthesis: An Investigation of Ion-Solid Interactions Under Extreme Processing Conditions" (invited paper)

International Conference on Strongly Correlated Electron Systems, Zürich, Switzerland, August 19–22, 1996:

K. Kempa, D. A. Broido, and H. H. Weitering, "Correlational Switching Between 3×1 and 6×1 Surface Reconstructions on Si(111) with Submonolayer Ag Adsorption"

American Chemical Society Meeting, Orlando, Florida, August 19–23, 1996:

A. R. Hopkins, P. G. Rasmussen, R. A. Basheer, B. K. Annis, and G. D. Wignall, "Analysis of Small-Angle Neutron Scattering (SANS) and Small-Angle X-Ray Scattering (SAXS) from Polyaniline Salts and Blends"

XXIIIth European Congress on Molecular Spectroscopy, Balatonfüred, Hungary, August 25–30, 1996:

O. Gamulin, M. Ivanda, U. Desnica, K. Furic, and T. E. Haynes, "Comparison of Structural Changes of Amorphous Silicon Induced by Thermal and CW Laser Annealing"

International Symposium on Metal Hydrogen Systems: Fundamentals and Applications, Les Diablerets, Switzerland, August 25–30, 1996:

H. K. Birnbaum, C. Buckley, S. Spooner, E. Sirois, F. Zeides, and J. S. Lin, "Hydrogen-Vacancy Interactions in Aluminum"

EUREM'96, Dublin, Ireland, August 26–30, 1996:

P. D. Nellist and S. J. Pennycook, "Incoherent Z-Contrast Imaging in a Coherent Microscope" (invited paper)

NATO Advanced Study Institute on Surface Diffusion: Atomistic and Collective Processes, Rhodes, Greece, August 26–September 6, 1996:

Z. Zhang, "Dynamics of Ad-Dimers at Surfaces" (invited paper)

International Materials Research Congress and Annual Meeting of the Mexican Association of Microscopy, Cancun, Mexico, September 1–5, 1996:

S. J. Pennycook, P. D. Nellist, and N. D. Browning, "Atomic Structure and Properties of Grain Boundaries in Ceramics Through Z-Contrast Electron Microscopy" (invited paper)

Tenth International Conference on Ion Beam Modification of Materials, Albuquerque, New Mexico, September 1–6, 1996:

L. A. Gea, L. A. Boatner, H. M. Evans, and R. A. Zuhr, "Optically Active Surfaces Formed by Ion Implantation and Thermal Treatment"

D. Ila, Z. Wu, C. C. Smith, and D. B. Poker, "Post Bombardment Enhanced Optical Absorption in Gold-Implanted Silica"

D. H. Lee, B. Park, and D. B. Poker, "Surface Hardness Enhancement in Ion-Implanted Amorphous Carbon"

A. Meldrum, L. M. Wand, R. C. Ewing, and L. A. Boatner, "Ion-Beam-Induced Amorphization of $LaPO_4$ and $ScPO_4$"

B. Nielsen and O. W. Holland, "Defects in Ion-Implanted Si Probed with Positrons"

Y. Qian, D. Ila, K. X. He, M. Curley, D. B. Poker, L. A. Boatner, and D. Hensley, "MeV Silver Ion Implantation Induced Changes in Optical Properties of MgO"

T. Taylor, D. Ila, R. L. Zimmerman, P. R. Ashley, D. B. Poker, and D. Hensley, "Optical Changes Induced in GaAs/AlGaAs Waveguides by MeV Ion Bombardment"

C. W. White, J. D. Budai, S. P. Withrow, J. G. Zhu, S. J. Pennycook, R. A. Zuhr, D. M. Hembree, Jr., D. O. Henderson, R. H. Magruder, III, M. J. Yacaman, G. Mondragon, and S. Prawer, "Encapsulated Nanocrystals and Quantum Dots Formed by Ion Beam Synthesis" (invited paper)

C. W. White, "Encapsulated Nanocrystals and Quantum Dots Formed by Ion Beam Synthesis" (invited paper)

E. K. Williams, D. Ila, S. Sarkisov, P. Venkateswarlu, D. B. Poker, D. Hensley, and T. R. Watkins, "MeV Ion-Beam-Assisted Fabrication of Buried Embedded Waveguides in Lithium Niobate"

E. K. Williams, D. Ila, S. Sarkisov, P. Venkateswarlu, and D. B. Poker, "Loss Measurements and Stoichiometric Dependence of Ti- and O-Implanted $LiNbO_3$ Waveguides"

J. M. Williams and D. B. Poker, "Ion Beam Mixing of Pt/Ti and Pt/Ni Bilayered Samples"

J. M. Williams and J. E. Miner, "Ion Implantation of Silicon Nitride Ball Bearings"

S. P. Withrow, C. W. White, J. D. Budai, J. G. Zhu, D. M. Hembree, Jr., and C. T. Olmstead, "Characterization of Si Nanocrystals Formed from a Uniform Si Implantation into SiO_2"

R. L. Zimmerman, D. Ila, D. B. Poker, and S. P. Withrow, "Permeability Control of GPC Drug Delivery Systems"

Fourth International Conference on Nanometer-Scale Science and Technology (NANO IV), Beijing, China, September 8–12, 1996:

Z. Zhang, "Patterning a Surface with Two-Dimensional Nanoislands" (invited paper)

Sixteenth European Conference on Surface Science, Genova, Italy, September 9–13, 1996:

K. Pohl and E. W. Plummer, "Greatly Enhanced Sensitivity to Hydrogen in LEED"

Tenth Alabama Materials Research Conference, Auburn, Alabama, September 18–19, 1996:

M. F. Chisholm, "Z-Contrast Imaging of Extended Defects in Semiconductors: A Technique of the Future?" (invited paper)

Royal Society of Chemistry Faraday Discussion Number 104: Complex Fluids at Interfaces, Cambridge, United Kingdom, September 18–20, 1996:

P. D. Butler, W. A. Hamilton, L. J. Magid, J. B. Hayter, T. M. Slawecki, and B. Hammouda "Use of Complementary Neutron Techniques in Studying the Effect of a Solid/Liquid Interface on Bulk Solution Structures" (invited paper)

International Conference on Physics of Transition Metals, Osaka, Japan, September 23–27, 1996:

R. S. Fishman, V. S. Viswanath, and S. H. Liu, "Spin and Charge Dynamics of Chromium Alloys" (invited paper)

Workshop on Determination of Morphology with Diffraction, Hilderheim, Germany, September 24–27, 1996:

J. F. Wendelken, A. K. Swan, H. Dürr, and J.-K. Zuo, "Morphology and Energy Barriers During Homoepitaxy on Cu(100)" (invited paper)

Nordic-Baltic Symposium on Nanostructures, Lithuania, September 27, 1996:

G. D. Mahan, "Thermoelectrics" (invited paper)

1996 IEEE International Silicon-On-Insulator Conference, Sanibel Island, Florida, September 30–October 3, 1996:

O. W. Holland and D. K. Sadana, "Technique to Form Ultrathin Buried Oxides in Si by O^+-Implantation"

M. K. Weldon, V. E. Marsico, Y. J. Chabal, S. B. Christman, E. E. Chaban, B. J. Sapjeta, D. J. Eaglesham, W. Brown, C. A. Goodwin, C. M. Hsieh, and A. Agarwal, "Mechanistic Studies of Hydrophilic Wafer Bonding and Si Exfoliation for SOI Fabrication"

International Semiconductor Conference CAS-96, Sinaia, Rumania, October 14–18, 1996:

S. T. Pantelides, M. Ramamoorthy, A. Maiti, M. F. Chisholm, and S. J. Pennycook, "Complex Impurity Dynamics in Silicon"

Tenth International Battery Association Battery Materials Symposium, Tucson, Arizona, October 1–4, 1996:

M. M. Thackeray, M. F. Mansuetto, and J. B. Bates, "Structural Stability of $LiMn_2O_4$ Electrodes for Lithium Batteries"

J. T. Zielke, M. Z. C. Hu, J. S. Lin, C. H. Byers, and M. T. Harris, "A Rapid Mixing Technique to Monitor the Hydrolysis and Condensation of Zirconium Butoxides and Titanium Ethoxides"

1996 Fall Meeting of the Physical Society of Japan, Yamaguchi, Japan, October 1–4, 1996:

M. Okada, A. P. Baddorf, and D. M. Zehner, "Hydrogen Adsorption on $Mo_{1-x}Re_x(110)$ (I)"

M. Okada, E. W. Plummer, A. P. Baddorf, and D. M. Zehner, "Hydrogen Adsorption on $Mo_{1-x}Re_x(110)$ (II)"

190th Meeting of the Electrochemical Society, San Antonio, Texas, October 6–11, 1996:

J. B. Bates, N. J. Dudney, and B. S. Kwak, "Sputter Deposition of $LiMn_2O_4$ Thin Films in Ar + N_2 Gas Mixtures"

J. B. Bates, B. Wang, and F. X. Hart, "Electrochemical Properties of $LiCoO_2$ in Thin-Film Lithium Cells"

N. D. Dudney, J. B. Bates, and F. X. Hart, "Hysteresis in the Lithium Insertion Reaction of Amorphous Cathodes"

B. J. Neudecker, R. A. Zuhr, B. S. Kwak, and J. D. Robertson, "Manganese-Substituted Lithium Nickel Oxide Thin-Film Cathodes"

First European Conference on Neutron Scattering, Interlaken, Switzerland, October 8–11, 1996:

A. T. Boothroyd, A. Mukherjee, S. Fulton, T. G. Perring, R. C. Eccleston, H. A. Mook, and B. M. Wanklyn, "High-Energy Magnetic Excitations in CuO"

International Symposium on Colloids and Polymer Science, Nagoya, Japan, October 10–13, 1996:

H. Seto, G. D. Wignall, R. Triolo, D. Chillura-Martino, and S. Komura, "Small-Angle Neutron Scattering Studies of Critical Phenomena of a Three-Component Microemulsion"

American Vacuum Society Forty Third National Symposium, Philadelphia, Pennsylvania, October 14–18, 1996:

D. B. Geohegan and A. A. Puretzky, "Advances in Pulsed-Laser Deposition Technology and Diagnostics" (invited paper)

D. O. Henderson, A. Ueda, R. Mu, Y. S. Tung, C. W. White, and J. G. Zhu, "Tin Implanted in Fused Silica: Optical Response from the Far-Infrared to the Ultraviolet" (invited paper)

J. A. Li, E. A. Akhadov, J. G. Skofronick, S. A. Safron, and L. A. Boatner, "Surface Structure and Dynamics of $KTaO_3$ by High-Resolution Helium Atom Scattering"

W. W. Pai, Z. Zhang, J. Zhang, and J. F. Wendelken, "Room-Temperature Molecular Manipulation with a Scanning Tunneling Microscope"

E. W. Plummer, A. T. Hanbicki, and K. Pohl, "The Dissociative Adsorption of Hydrogen: From Simple Metals to Alloys" (invited paper)

K. Pohl, P. Hofmann, S. V. Christensen, and E. W. Plummer, "The Bonding Configuration and Phase Diagram of the H/Be(0001) System"

Z.-P. Shi and Z. Zhang, "Effects of Dimer Shearing in Heteroepitaxy and Dimer Sliding Along Step Edges on Metal (100) Surfaces"

Fifth Annual Workshop of the Consortium for Nanostructured Materials," Nashville, Tennessee, October 18–19, 1996:

J. D. Budai, "Synthesis and Structure of Ion-Implanted Nanocrystals" (invited paper)

Forty-Seventh Annual Gaseous Electronics Conference, Argonne, Illinois, October 20–24, 1996:

C. Doughty and S. M. Gorbatkin, "Deposition of Ultrahard Coatings in a Plasma Environment" (invited paper)

D. B. Geohegan, A. A. Puretzky, R. F. Wood, and J.-N. Leboeuf, "Dynamics of Laser Ablation Plasmas in Vacuum and Background Gases: Effects of Scattering and Interplume Collisions on Velocity Distributions Used for PLD Film Growth" (invited paper)

Ninth International Symposium on Superconductivity, ISS'96, Sapporo, Hokkaido, Japan, October 21–24, 1996.

A. Goyal, D. P. Norton, M. Paranthaman, J. D. Budai, E. D. Specht, D. K. Christen, D. M. Kroeger, Q. He, B. Saffian, F. A. List, D. Lee, C. Klabunde, and P. Martin, "Fabrication of High Critical Current Density Superconducting Tapes by Epitaxial Deposition of YBaCuO Thick Films on Biaxially Textured Metal Substrates"

M. Paranthaman, A. Goyal, D. P. Norton, F. A. List, E. D. Specht, D. K. Christen, D. M. Kroeger, J. D. Budai, Q. He, B. Saffian, D. Lee, and P. Martin, "Development of Biaxially Textured Buffer Layers on Rolled-Ni Substrates for High-Current $YBa_2Cu_3O_{7-\gamma}$ Coated Conductors"

Fifteenth Annual Symposium on Advances in Microscopy, Wrightsville Beach, North Carolina, October 25–27, 1996:

S. J. Pennycook, P. D. Nellist, M. F. Chisholm, D. J. Wallis, and N. D. Browning, "Z-Contrast Imaging in Materials Science" (invited paper)

Symposium of Northeastern Accelerator Personnel, Woods Hole, Massachusetts, October 27, 1996:

D. K. Hensley, "1996 Laboratory Report to Symposium of Northeastern Accelerator Personnel for the Surface Modification and Characterization Research Center at Oak Ridge National Laboratory"

Ninth National Congress of Polymers in Mexico, Mexico City, Mexico, October 28–31, 1996:

F. J. Medellin-Rodriguez, C. A. Avila-Orta, L. Larios-Lopez, and J. S. Lin, "Interfacial Morphology of Nylon 6 by Means of Small-Angle X-Ray Scattering"

The American Ceramic Society Fall Meeting, San Antonio, Texas, October 30–November 2, 1996:

B. C. Sales and L. A. Boatner, "High-Performance Liquid Chromatography Investigations of Intermediate-Range Order in Amorphous Phosphates" (invited paper)

B. C. Sales, L. A. Boatner, J. O. Ramey, J. U. Otaigbe, and C.-K. Loong, "Structural Investigations of Intermediate-Range Order in Zinc Phosphate Glasses"

Second International Symposium on Ionizing Radiation and Polymers, Guadeloupe, France, November 3, 1996:

D. Ila, R. L. Zimmerman, G. M. Jenkins, D. B. Poker, and S. P. Withrow, "The Absorption of Lithium Salt in Polymeric Carbons"

Fourteenth International Conference on the Application of Accelerators in Research and Industry, Denton, Texas, November 6–9, 1996:

C. Doughty and S. M. Gorbatkin, "Metallization from High-Density Plasmas" (invited paper)

A. L. Evelyn, D. Ila, R. L. Zimmerman, K. Bhat, D. B. Poker, and D. K. Hensley, "Resolving the Effects of the Electronic and Nuclear Stopping Powers in MeV-Irradiated Polymer Films"

T. Taylor, D. Ila, R. L. Zimmerman, P. R. Ashley, D. B. Poker, and D. K. Hensley, "Effects of Substrate Temperature on the Fabrication of Optical Channels in Planar GaAs/AlGaAs Waveguides Using MeV Ions"

R. L. Zimmerman, D. Ila, D. B. Poker, and S. P. Withrow, "Ion Beam Processing of Drug Delivery Systems" (invited paper)

SERMACS '96, Greenville, South Carolina, November 10–13, 1996:

P. D. Butler, "Effect of Mixed Counterions on the Behavior of Surfactant Solutions Under Shear" (invited paper)

Annual Meeting of the American Institute of Chemical Engineering, Chicago, Illinois, November 10–15, 1996:

M. Z. C. Hu, J. T. Zielkie, M. T. Harris, J. S. Lin, and C. H. Byers, "Nucleation and Growth Kinetics for Synthesis of Nonometric Zirconia Particles"

A. Singhal, M. T. Harris, M. Z. Hu, L. M. Toth, and J. S. Lin, "Small-Angle X-Ray Scattering Study on Zirconium Hydrous Polymers in Organic Solutions"

J. T. Zielke, M. Z. C. Hu, J. S. Lin, C. H. Byers, and M. T. Harris, "A Rapid Mixing Technique to Monitor the Hydrolysis and Condensation of Zirconium Butoxides and Titanium Ethoxides"

41st Annual Conference on Magnetism and Magnetic Materials, Atlanta, Georgia, November 12–15, 1996:

P. Dai, J. A. Fernandez-Baca, B. C. Chakoumakos, J. Cable, S. E. Nagler, P. Schiffer, N. Kalechfsky, M. Roy, Y.-K. Tsui, P. J. McGinn, S. L. Einloth, and A. P. Ramirez, "Structural and Magnetic Properties of $La_{0.5}Ca_{0.5}MnO_3$"

J. A. Fernandez-Baca, E. Fawcett, H. L. Alberts, V. Y. Galkin, and Y. Endoh, "Effect of Pressure on the Magnetic Phase Diagram of the Antiferromagnetic Spin-Density-Wave Alloy Cr-1.6% Si"

R. S. Fishman and X. W. Jiang, "Charge-Density Wave and Magnetic Phase Diagram of Chromium Alloys"

A. W. Garrett, S. E. Nagler, T. Barnes, and B. C. Sales, "Excitations in the Spin Ladder Material $(VO)_2P_2O_7$"

D. Mandrus, J. L. Sarrao, B. C. Chakoumakos, J. A. Fernandez-Baca, S. E. Nagler, and B. C. Sales, "Magnetism in $BaCoS_2$"

Z.-P. Shi, Y. Wang, and G. M. Stocks, "*Ab Initio* Study of Biquadratic Coupling in Fe/Cr Multilayers"

Southeast Section of the American Physical Society, Decatur, Georgia, November 14, 1996:

S. T. Pantelides, "Complex Atom Dynamics in Solids" (invited paper)

S. T. Pantelides, M. Ramamoorthy, A. Maiti, M. F. Chisholm, and S. J. Pennycook, "Complex Impurity Dynamics in Silicon"

Dinner Meeting of the East Tennessee Section of the Materials Research Society, Knoxville, Tennessee, November 19, 1996:

G. D. Wignall, "Neutrons and Polymers: Why Do They Mix So Well?" (invited paper)

Integration of Interdisciplinary Materials Research, North Carolina Materials Research Society, Research Triangle Park, North Carolina, November 22, 1996:

G. D. Wignall, "Miscibility and Segregation in Blends of Linear and Branched Polymers" (invited paper)

The Department of Energy Center of Excellence for the Synthesis and Processing of Advanced Materials, Advanced Photovoltaic Project, Lakewood, Colorado, November 22, 1996:

G. Eres, D. H. Lowndes, and D. C. Lubben, "Low-Temperature Epitaxy of Thick Silicon Films" (invited paper)

D. H. Lowndes, C. M. Rouleau, and J. D. Budai, "Epitaxial Growth of $CuInSe_2$ and Other I-III-VI_2 Materials by Pulsed-Laser Ablation" (invited paper)

STCS-CNRS Workshop in Superconductivity, Evanston, Illinois, November 25, 1996:

D. K. Christen, "Superconducting Transport Properties of High-J_c $YBa_2Cu_3O_{7-\delta}$ Thick Films Deposited on Biaxially Oriented Metallic Substrates" (invited paper)

Fall Meeting of the Materials Research Society, Boston, Massachusetts, December 2–6, 1996:

M. M. Agamalian, G. D. Wignall, R. G. Alamo, J. D. Londono, L. Mandelkern, and F. C. Stehling, "Ultrahigh Resolution Small-Angle Neutron Scattering Investigations of Liquid-Liquid Phase Separation in Linear Low-Density Polyethylene"

A. Agarwal, T. E. Haynes, D. J. Eaglesham, D. C. Jacobson, H. J. Gossman, J. M. Poate, and Y. Erokhin, "Damage, Defects, and Diffusion from 1–5-keV Implants in Silicon"

R. A. Brown, G. A. Rozgonyi, J. Ravi, Y. Erokhin, and C. W. White, "Charge State Defect Engineering of Silicon During Ion Implantation"

N. D. Browning, D. J. Wallis, and S. J. Pennycook, "Determination of the Three-Dimensional Atomic Structure at Internal Interfaces by Electron Energy Loss Spectroscopy"

J. D. Budai, C. W. White, S. P. Withrow, R. A. Zuhr, and J. G. Zhu, "Synthesis, Optical Properties, and Microstructure of Semiconductor Nanocrystals Formed by Ion Implantation" (invited paper)

M. F. Chisholm, T. Kaplan, M. Mostoller, and S. J. Pennycook, "Structure and Properties of Dislocations and Grain Boundaries in Silicon"

D. K. Christen, D. P. Norton, A. Goyal, J. D. Budai, Q. He, C. E. Klabunde, D. M. Kroeger, D. F. Lee, F. A. List, M. Paranthaman, B. Saffian, and E. D. Specht, "Superconducting Transport Properties of High-J_c $YBa_2Cu_3O_{7-\delta}$ Thick Films Deposited on Biaxially Oriented Metallic Substrates" (invited paper)

E. C. Dickey, V. P. Dravid, S. J. Pennycook, P. D. Nellist, and D. J. Wallis, "A Combined Techniques Approach to Elucidating Crystalline Interface Atomic Structure"

A. L. Evelyn, D. Ila, R. L. Zimmerman, K. Bhat, D. B. Poker, and D. K. Hensley, "Effects of MeV Ion Beam on Polymers"

R. Feenstra, T. Matsumoto, and T. Kawai, "Doping of the Copper-Oxygen Planes in the Near-Surface Region Studied by Scanning Tunneling Spectroscopy"

D. O Henderson, R. Mu, A. Ueda, C. W. White, J. G. Zhu, and J. D. Budai, "Gold Implanted in Porous Glass: Size and Shape Effects on the Surface Plasmon Absorption of Gold Nanocrystals"

D. O. Henderson, R. Mu, A. Ueda, Y.-S. Tung, C. W. White, J. G. Zhu, and J. D. Budai, "Size Control of Indium Phosphide Quantum Dots Formed by Sequential Ion Implantation of Phosphorous and Indium Porous Vycor Glass"

D. O. Henderson, R. Mu, A. Ueda, Y.-S. Tung, C. W. White, J. G. Zhu, and J. D. Budai, "Optical and Structural Characterization of Zinc-Implanted Silica Under Various Thermal Treatments"

J. J. Hoyt, B. C. Chakoumakos, S. T. Misture, R. McCormack, and M. D. Asta, "X-Ray and Neutron Scattering Study of the Order-Disorder Transition in $AlMnCu_2$"

F. Hui and G. Eres, "Advanced Lithography of Nanofabrication"

D. Ila, Y. Qian, Z. Wu, C. C. Smith, D. B. Poker, and D. K. Hensley, "Application of MeV Ion Implantation in the Formation of Nano-Metallic Clusters in Photorefractive Materials"

D. Ila, Y. Qian, Z. Wu, M. Curley, D. B. Poker, and D. K. Hensley, "Formation of Silver Metal Nanoclusters in MgO by MeV Ag Implantation"

D. Ila, Z. Wu, C. C. Smith, D. B. Poker, and D. K. Hensley, "Post Bombardment Enhanced Optical Absorption in Gold-Implanted Suprasil Silica"

D. E. Jesson, K. M. Chen, S. J. Pennycook, T. Thundat, and R. J. Warmack, "Kinetic Pathways for the Stress-Driven 2D-to-3D Transition"

A. A. Jones, P. T. Inglefield, C. Zhang, P. Bergquist, J. Shi, R. P. Kambour, G. D. Wignall, H. Migeon, and J. Martin, "Morphology of a Blend of Zinc-Neutralized Sulfonated Poly(Phenylene Oxide) of Polystyrene and an Amino Silicone"

T. Kaplan, F. Liu, M. Mostoller, and M. F. Chisholm, "First-Principles Study of Dislocations in Silicon: Impurity Segregation"

V. M. Keppens, D. Mandrus, J. Rankin, and L. A. Boatner, "The Formation of Metal/Metal-Matrix Nano-Composites by the Ultrasonic Dispersion of Immiscible Liquid Metals"

H. R. Kerchner, D. K. Christen, J. R. Thompson, and T. Armstrong, "Angular Study of $YBa_2Cu_3O_{7-\delta}$ Magnetic Hysteresis"

A. Maiti, M. F. Chisholm, S. J. Pennycook, and S. T. Pantelides, "Cooperative Chemical Rebonding in the Segregation of Impurities in Silicon Grain Boundaries" (invited paper)

R. H. Magruder, III, R. A. Weeks, T. S. Anderson, and R. A. Zuhr, "Linear and Nonlinear Optical Properties of Metal Nanocluster-Silica Composites Formed by Implantation of Sb in High-Purity Silica"

D. W. Marr, K. B. Schwartz, G. D. Wignall, and M. M. Agamalian, "Void Morphology in Polyethyene/Carbon Black Composites"

P. C. Mason, B. D. Gaulin, R. M. Epand, G. D. Wignall, and J. S. Lin, "Coherent and Incoherent Ripples in Dipalmitoylphosphatidylcoline"

A. Meldrum, L. A. Boatner, and R. C. Ewing, "Electron-Irradiation-Induced Crystallization of Amorphous Orthophosphates"

R. Mu, J. Chen, Z. Y. Gu, A. Ueda, T. S. Tung, D. O. Henderson, C. W. White, J. G. Zhu, J. D. Budai, and R. A. Zuhr, "Optical and Structural Characterization of Zinc-Implanted Silica under Various Thermal Treatments"

D. P. Norton, A. Goyal, J. D. Budai, D. K. Christen, D. M. Kroeger, E. D. Specht, Q. He, B. Saffian, M. Paranthaman, C. E. Klabunde, D. F. Lee, B. C. Sales, and F. A. List, "Epitaxial Growth of $YBa_2Cu_3O_7$ on Biaxially Textured (001) Ni" (invited paper)

S. J. Pennycook, N. D. Browning, P. D. Nellist, M. F. Chisholm, and D. P. Norton, "Toward the Atomic Level Engineering of Grain Boundaries in Ceramic Superconductors" (invited paper)

S. J. Pennycook, P. D. Nellist, M. F. Chisholm, N. D. Browning, D. J. Wallis, and E. C. Dickey, "Determination of Atomic Structure at Surfaces and Interfaces by High-Resolution STEM" (invited paper)

Y. S. Tung, R. Mu, A. Ueda, D. O. Henderson, P. W. Wang, C. W. White, J. G. Zhu, and R. A. Zuhr, "Carbon Implanted in Optical Grade Fused Silica: Annealing Effects in Reducing and Oxidizing Atmospheres"

K. C. Walter, J. M. Williams, J. S. Woodring, M. Nastasi, D. B. Poker, and C. P. Munson, "Properties of Ion-Implanted Ti-6Al-4V Processed Using Beam Line and PSII Techniques"

J. G. Zhu, C. W. White, J. D. Budai, S. P. Withrow, R. Mu, and D. O. Henderson, "Ion Beam Modification of Optical Materials and Synthesis of Semiconductor Nanocrystals"

R. A. Zuhr, R. H. Magruder, III, and T. S. Anderson, "Optical Properties of Multicomponent Cadmium-Silver Nanocluster Composites Formed in Silica by Sequential Ion Implantation"

International Conference on Stripes, Lattice Instabilities, and High-T_c Superconductivity, Rome, Italy, December 8–12, 1996:

H. A. Mook and B. C. Chakoumakos, "Incommensurate Fluctuations in $Bi_2Sr_2CaCu_2O_8$" (invited paper)

Condensed Matter and Material Physics Conference, York, United Kingdom, December 17–19, 1996:

D. A. Tennant, S. E. Nagler, A. W. Garrett, T. Barnes, C. Torardi, A. C. I. Lake, and R. A. Cowley, "Magnetic Superexchange Through Covalent Bridges in Spin Dimer Compound $(VO)DPO_4 \bullet 0.5D_2O$ and Alternating Chain Compound $CuWO_4$" (invited paper)

Winter Workshop on Atomic Structure and Chemistry of Interfaces, Tempe, Arizona, January 7–11, 1997:

S. J. Pennycook, M. F. Chisholm, P. D. Nellist, A. Maiti, and S. T. Pantelides, "Probing Structure Property Relationships at Interfaces by Atomic-Resolution Z-Contrast Imaging, EELS, and Theory" (invited paper)

Fifth International Conference on Polymer Characterization, Denton, Texas, January 8–10, 1997:

W.-C. Ko, H.-H. Wang, Y.-J. Hu, and J. S. Lin, "Small-Angle X-Ray Scattering of Poly(ethylene Terephthalate) Multifilaments from Spin-Draw Process: Effect of Processing Conditions"

International Conference of Condensed Matter Physics (ICCMP), Brasilia, Brazil, February 24–28, 1997:

R. S. Fishman, "Properties of Spin-Density Wave Systems" (invited paper)

Workshop on Quantitative Methods in Materials Research, Santa Barbara, February 4, 1997:

Z. Zhang, "Atomistic View of Two-Dimensional Pattern Formation in Epitaxial Growth: Fractals, Dendrites, and Compact Islands" (invited paper)

Low-Energy Beam Processes in Electronic Materials, The Metallurgical Society, Orlando, Florida, February 9–13, 1997:

D. P. Norton, "Role of Energetic Species in Laser Ablation Film Growth" (invited paper)

126th TMS Annual Meeting and Exhibition, Orlando, Florida, February 9–13, 1997:

E. G. Roth and O. W. Holland, "Defect-Engineered Shallow Junctions" (invited paper)

Optical Society of America Winter Topical Meeting, Santa Fe, New Mexico, February 9–16, 1997:

G. Eres and F. Y. C. Hui, "Advanced Lithography for Nanofabrication"

Symposium on Evolution and Advanced Characterization of Thin-Film Microstructures, Orlando, Florida, February 10–12 1997:

D. E. Jesson, "New Insights into the Stress-Driven 2D-to-3D Transition" (invited paper)

NASA University Research Centers Technical Conference, Albuquerque, New Mexico, February 16–19, 1997:

Y. S. Tung, D. O. Henderson, R. Mu, A. Ueda, W. E. Collins, C. W. White, R. A. Zuhr, and J. G. Zhu, "Au Colloids Formed by Ion Implantation in Muscovite Mica Studied by Vibrational and Electronic Spectroscopies and Atomic Force Microscopy"

A. Ueda, R. Mu, T. S. Tung, D. O. Henderson, C. W. White, R. A. Zuhr, J. G. Zhu, and P. W. Wang, "Annealing Effects on the Surface Plasmon of MgO Implanted with Gold"

J. G. Zhu, C. W. White, S. P. Withrow, J. D. Budai, and D. O. Henderson, "Ion Beam Synthesis and Optical Properties of Semiconductor Nanocrystals and Quantum Dots"

97 WATTec Conference, Knoxville, Tennessee, February 24–26, 1997:

J. B. Bates, "Thin-Film Rechargeable Lithium Batteries" (invited paper)

Fifth International Conference on Materials and Mechanisms of Superconductivity—High-Temperature Superconductors V, Beijing, China, February 28–March 4, 1997:

R. Feenstra, T. Matsumoto, and T. Kawai, "Scanning Tunneling Microscopy and Spectroscopy Study of Substitution- and Defect-Doped Films of the Infinite-Layer Compound" (invited paper)

International Workshop on Critical Currents in Superconductors for Practical Applications (SPA '97), Xian, China, March 6–8, 1997:

D. K. Christen, D. P. Norton, A. Goyal, J. D. Budai, R. Feenstra, Q. He, C. E. Klabunde, D. M. Kroeger, D. F. Lee, F. A. List, M. Paranthaman, B. Saffian, E. D. Specht, and M. F. Chisholm, "Fabrication and Properties of High-J_c Biaxially Aligned $YBa_2Cu_3O_{7-\delta}$ Thick Films on Metallic Tape Substrates" (invited paper)

March Meeting of the American Physical Society, Kansas City, Missouri, March 17–21, 1997:

B. K. Annis, G. D. Wignall, A. R. Hopkins, P. G. Rasmussen, and R. A. Basheer, "Structural Investigation of Polyaniline (PANI)/Nylon 6 Blends by Small-Angle Neutron Scattering (SANS) and Small- and Wide-Angle X-Ray Scattering (SAXS and WAXS)" [*Bull. Am. Phys. Soc.* **42**, 587 (1997)]

A. P. Baddorf, V. Jahns, E. W. Plummer, and J. Zhang, "Structure and Dynamics of the Sn/Ge(111) CDW" [*Bull. Am. Phys. Soc.* **42**, 557 (1997)]

M. Bartkowiak and G. D. Mahan, "Dynamics of Two-Dimensional Topologically Disordered Josephson Arrays" [*Bull. Am. Phys. Soc.* **42**, 121 (1997)]

J. D. Budai, C. W. White, S. P. Withrow, R. A. Zuhr, and J. G. Zhu, "Microstructure and Properties of Semiconductor Nanocrystals Formed by Ion Implantation" [*Bull. Am. Phys. Soc.* **42**, 406 (1997)]

J. M. Carpinelli, "Charge Ordering Transitions in Thin Films of Pb and Sn on Ge(111)" [*Bull. Am. Phys. Soc.* **42**, 704 (1997)] (invited paper)

D. K. Christen, D. P. Norton, A. Goyal, J. D. Budai. Q. He, C. E. Klabunde, R. Feenstra, D. M. Kroeger, D. F. Lee, F. A. List, M. Paranthaman, B. Saffian, E. D. Specht, and M. F. Chisholm, "Superconducting Properties of High-J_C Biaxially Aligned $YBa_2Cu_3O_{7-\delta}$ Thick Films on Metallic Tape Substrates" [*Bull. Am. Phys. Soc.* **42**, 293 (1997)]

J. F. Cooke and J. A. Blackman, "Theoretical Investigation of the Orbital Contribution to Inelastic Neutron Scattering Cross Sections for Transition-Metal Ferromagnets" [*Bull. Am. Phys. Soc.* **42**, 620 (1997)]

R. Feenstra, T. Matsumoto, and T. Kawai, "Scanning Tunneling Microscopy/Spectroscopy (STM/STS) Study of Doping Properties in the Infinite-Layer Compound" [*Bull. Am. Phys. Soc.* **42**, 481 (1997)]

J. A. Fernandez-Baca, P. Dai, S. E. Nagler, B. C. Chakoumakos, J. W. Cable, P. Schiffer, N. Kalechfsky, M. Roy, Y.-K. Tsui, P. J. McGinn, S. L. Einloth, and A. P. Ramirez, "Structural and Magnetic Properties of $La_{0.5}Ca_{0.5}MnO_3$" [*Bull. Am. Phys. Soc.* **42**, 321 (1997)]

R. S. Fishman and V. S. Viswanath, "Density of States in Chromium Alloys" [*Bull. Am. Phys. Soc.* **42**, 732 (1997)]

D. B. Geohegan and A. A. Puretzky, "Laser Ablation Plume Dynamics Relevant to Materials Synthesis and Analysis" [*Bull. Am. Phys. Soc.* **42**, 95 (1997)] (invited paper)

A. Hanbicki and E. W. Plummer, "The Face-Dependent Interaction of Hydrogen with NiAl" [*Bull. Am. Phys. Soc.* **42**, 252 (1997)]

A. R. Hopkins, P. G. Rasmussen, R. A. Basheer, B. K. Annis, and G. D. Wignall, "Analysis of Small-Angle Neutron Scattering (SANS) and Small-Angle X-Ray Scattering (SAXS) from Polyaniline Salts and Blends"

P. Hyldgaard and G. D. Mahan, "Dramatic High-Temperature Suppression of Perpendicular Heterostructure-Phonon Transport" [*Bull. Am. Phys. Soc.* **42**, 218 (1997)]

Ismail, P. Hofmann and E. W. Plummer, "Phonon Dispersion at the Mg(0001) Surface" [*Bull. Am. Phys. Soc.* **42**, 136 (1997)]

V. Jahns, D. M. Zehner, G. Watson, and L. D. Gibbs, "Ir(001) Surface Structure Determination by X-Ray Scattering" [*Bull. Am. Phys. Soc.* **42**, 135 (1997)]

D. E. Jesson, "Morphological Evolution of the Stress-Driven Two-Dimensional to Three-Dimensional Transition" [*Bull. Am. Phys. Soc.* **42**, 226 (1997)] (invited paper)

K.-J. Jin, S.-H. Pan, G.-Z. Yang, and G. D. Mahan, "Simulation of Morphological Evolution and RHEED Intensity Oscillations During Thin-Film Growth" [*Bull. Am. Phys. Soc.* **42**, 687 (1997)]

B. C. Larson, "Inelastic X-Ray Scattering Measurement of the Many-Body Local-Field Factor in a Simple Metal" [*Bull. Am. Phys. Soc.* **42**, 622 (1997)] (invited paper)

J. A. Li, J. Baker, E. Akhadov, T. Trelenberg, J. G. Skofronick, S. A. Safron, and L. A. Boatner, "The Structure of the Perovskite $KTaO_3$ Surface by Helium Atom Surface Scattering" [*Bull. Am. Phys. Soc.* **42**, 340 (1997)]

J. S. Lin, J. D. Londono, G. D. Wignall, H. D. Cochran, A. I. Cooper, J. B. McClain, J. M. DeSimone, and J. M. Frechet, "Structure of Unimolecular Dendritic Reverse Micelle in Dense Carbon Dioxide via Small-Angle Scattering" [*Bull. Am. Phys. Soc.* **42**, 794 (1997)] (invited paper)

K. C. Lin, H. H. Weitering, O. W. Holland, and L. C. Feldman, "Surface Characterization of SOI Materials" [*Bull. Am. Phys. Soc.* **42**, 378 (1997)]

A. Maiti, G. D. Mahan, and S. T Pantelides, "Dynamical Simulations of Nonequilibrium Processes—Heat Flow and the Kapitza Resistance Across Grain Boundaries" [*Bull. Am. Phys. Soc.* **42**, 692 (1997)]

D. C. Marinescu, "Thermoelectric Flux in Superconducting Rings—A Search for a Factor of 10^5" [*Bull. Am. Phys. Soc.* **42**, 66 (1997)] (invited paper)

D. C. Marinescu and J. J. Quinn, "Local Field Corrections to the RPA Response Functions of a Spin-Polarized Electron Gas" [*Bull. Am. Phys. Soc.* **42**, 675 (1997)]

D. C. Marinescue, S. Yi, P. Sitko, and J. J. Quinn, "Composite Fermions and the Half-Filled State" [*Bull. Am. Phys. Soc.* **42**, 342 (1997)]

S. E. Nagler, "Magnetic Excitations in $(VO)_2P_2O_7$" [*Bull. Am. Phys. Soc.* **42**, 286 (1997)] (invited paper)

S. E. Nagler and B. C. Chakoumakos, "Polarized Neutron Diffraction Study of $SrRuO_3$" [*Bull. Am. Phys. Soc.* **42**, 551 (1997)]

B. Nielsen, P. Asoka-Kumar, O. W. Holland, T. E. Haynes, E. Roth, and V. C. Venezia, "Vacancy Clustering and Vacancy Impurity Interactions in Si" [*Bull. Am. Phys. Soc.* **42**, 792 (1997)]

D. P. Norton, C. Park, and J. D. Budai, "Effect of Energetic Ions on Cerium Oxide Films Deposited by Pulsed-Laser Deposition" [*Bull. Am. Phys. Soc.* **42**, 42 (1997)]

W. W. Pai, J. F. Wendelken, J. Zhang, and E. W. Plummer, "Friedel Oscillations on Metal Surfaces Induced by Bulk State Electrons" [*Bull. Am. Phys. Soc.* **42**, 28 (1997)]

W. W. Pai, Z. Zhang, J. Zhang, and J. F. Wendelken, "Room-Temperature STM Manipulation of Stable Radicals with a Novel Mechanism" [*Bull. Am. Phys. Soc.* **42**, 707 (1997)]

S. J. Pennycook, M. F. Chisholm, P. D. Nellist, A. Maiti, and S. T. Pantelides, "High-Resolution Scanning Transmission Electron Microscopy" [*Bull. Am. Phys. Soc.* **42**, 111 (1997)] (invited paper)

K. Pohl and E. W. Plummer, "Temperature-Dependent Interplanar Spacing of the (0001) Surface of Beryllium" [*Bull. Am. Phys. Soc.* **42**, 137 (1997)]

C. M. Rouleau, D. H. Lowndes, and J. D. Budai, "Pulsed-Laser Deposition of Epitaxial $CuInSe_2$ on GaAs" [*Bull. Am. Phys. Soc.* **42**, 216 (1997)]

B. C. Sales, "Filled Skutterudite Antimonides: A New Class of Thermoelectric Materials" [*Bull. Am. Phys. Soc.* **42**, 272 (1997)] (invited paper)

I. Sandler, G. Canright, and Z. Zhang, "Spontaneous Chiral Symmetry Breaking in 2D Aggregation: A Continuum Model" [*Bull. Am. Phys. Soc.* **42**, 338 (1997)]

C.-K. Shih, A. R. Smith, K.-J. Chao, Q. Niu, and Z. Zhang, "Flattening Metallic Thin Films on Non-Wetting Semiconductor Substrates" [*Bull. Am. Phys. Soc.* **42**, 686 (1997)]

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Z.-P. Shi and R. S. Fishman, "Interplay Between Spin Density Wave and Proximity Magnetic Layers" [*Bull. Am. Phys. Soc.* **42**, 141 (1997)]

J. O. Sofo, M. Bartkowiak, and G. D. Mahan, "First-Principles Study of Se-Intercalated Graphite" [*Bull. Am. Phys. Soc.* **42**, 22 (1997)]

A. Tennant, S. E. Nagler, A. W. Garrett, T. Barnes, and C. Torardi, "Inelastic Neutron Scattering Study of Magnetic Excitations in the Spin Dimer $(VO)DPO_4 \bullet 0.5D_2O$" [*Bull. Am. Phys. Soc.* **42**, 621 (1997)]

J. R. Thompson, "Superfast Vortex Creep at Low Fields in YBCO Single Crystals with Columnar Defects" [*Bull. Am. Phys. Soc.* **42**, 422 (1997)] (invited paper)

J. Z. Tischler, B. C. Larson, A. G. Eguiluz, and A. Fleszar, "The ω Dependence of the Many-Body Local-Field Factor in Al" [*Bull. Am. Phys. Soc.* **42**, 778 (1997)]

J. F. Wendelken, W. W. Pai, A. K. Swan, and Z. Zhang, "Cluster Diffusion and Coarsening in Cu(001) Homoepitaxy" [*Bull. Am. Phys. Soc.* **42**, 687 (1997)]

L. Woods and G. D. Mahan, "Nonlinear Electron-Phonon Heat Exchange" [*Bull. Am. Phys. Soc.* **42**, 674 (1997)]

J. Zhang, Ismail, J. M. Carpinelli, and E. W. Plummer, "Surface Charge Density Wave Induced Lattice Distortion: A LEED Study of the SN/Ge(111) and Pb/Ge(111) Systems" [*Bull. Am. Phys. Soc.* **42**, 558 (1997)]

Z. Zhang and Q. Niu, "Quantum Mechanically Defined Critical Thickness in Metallic Overlayer Heteroepitaxy" [*Bull. Am. Phys. Soc.* **42**, 686 (1997)]

J.-K. Zuo and J. F. Wendelken, "Evolution of Mound Morphology in Reversible Homoepitaxy on Cu(100)" [*Bull. Am. Phys. Soc.* **42**, 576 (1997)]

First Conference on Future Generation Photovoltaic Technologies, Denver, Colorado, March 24–26, 1997:

D. P. Norton, J. D. Budai, A. Goyal, D. H. Lowndes, D. M. Kroeger, D. K. Christen, M. Paranthaman, and E. D. Specht, "Low-Cost Metal Substrates for Films with Aligned Grain Structures" (invited paper)

International Conference on Surface Physics and Thin Films, Taipei, Taiwan, March 25–28, 1997:

Z. Zhang, "Toward Quantum Engineering of Ultrathin Metallic Overlayers on Semiconductor Substrates" (invited paper)

Spring Meeting of the Materials Research Society, San Francisco, California, March 31–April 4, 1997:

A. Agarwal, D. J. Eaglesham, H. J. Gossmann, T. E. Haynes, D. C. Jacobson, Y. Erokhin, and J. M. Poate, "New Aspects of Very Low Energy Ion-Implantation for Ultrashallow Junctions" (invited paper)

D. K. Christen, D. P. Norton, A. Goyal, J. D. Budai, Q. He, C. E. Klabunde, D. M. Kroeger, D. F. Lee, F. A. List, M. Paranthaman, B. Saffian, E. D. Specht, and M. F. Chisholm, "Superconducting Properties of High-J_c Biaxially Aligned $YBa_2Cu_3O_{7-\delta}$ Thick Films on Metallic Tape Substrates" (invited paper)

H.-M. Christen, D. G. Mandrus, D. P. Norton, L. A. Boatner, and B. C. Sales, "Properties of $CoSb_3$ Films Grown by Pulsed-Laser Deposition"

D. J. Eaglesham, D. Huber, D. C. Jacobson, K. Bourdelle, A. Agarwal, J. L. Benton, J. M. Poate, R. Dulas, S. Wilson, Y. Erokhin, L. Rubin, J. Sedgewick, and S. Saito, "MeV Implants for Gettering in Silicon"

H.-J. Gossmann, T. E. Haynes, P. A. Stolk, T. K. Mogi, C. A. King, R. W. Johnson, D. C. Jacobson, H. S. Luftman, M. O. Thompson, and J. M. Poate, "Diffusion of Common Dopants in Si: The Interstitial Fraction"

T. Isobe, R. A. Weeks, and R. A. Zuhr, "Magnetic Properties of Nanosize Particles Produced in Silica Glasses by Implanting Ni^+ and $N^+ + Fe^+$"

D. E. Jesson, G. Y. Chen, K. M. Chen, S. J. Pennycook, T. Thundat, and R. J. Warmack, "Mechanisms of Morphological Evolution During Strained-Layer Epitaxy" (invited paper)

D. Mandrus, B. C. Sales, V. Keppens, B. C. Chakoumakos, P. Dai, L. A. Boatner, R. K. Williams, J. R. Thompson, T. W. Darling, A. Migliori, M. B. Maple, D. A. Gajewski, and E. J. Freeman, "Filled Skutterudite Antimonides: Validation of the Electron-Crystal Phonon-Glass Approach to New Thermoelectric Materials" (invited paper)

B. Nielsen, O. W. Holland, P. Asoka-Kumar, E. Roth, and V. Venezia, "Vacancy Impurity Interactions in Si"

D. P. Norton, C. Park, B. Saffian, J. D. Budai, A. Goyal, D. K. Christen, D. M. Kroeger, D. F. Lee, and Q. He, "Epitaxial Growth of Oxide Thin Films on (001) Metal Surfaces using Pulsed-Laser Deposition"

V. C. Venezia, T. E. Haynes, A. Agarwal, H.-J. Gossmann, and D. J. Eaglesham, "Enhanced Diffusion of Dopants in Vacancy Supersaturations Produced by MeV Implantation"

Seminars

SOLID STATE DIVISION SEMINARS AT ORNL

During this period B. C. Sales served as Seminar Chairman assisted by L. W. Hinton, April 1995–continuing. The following seminars were held:

"What Materials Research Do We Really Need for Si Industry?" J. M. Poate, AT&T Bell Laboratories, Murray Hill, N.J.

"Dielectric Properties of Sputtered $SrTiO_3$ Thin Films," H.-M. Christen, Swiss National Science Foundation, Lausanne, Switzerland

"Thermodynamic and Structural Properties of Polymer Blends and Solutions in the Region of Critically Fluctuating Order Parameters," Y. Melnichenko, Max-Planck-Institut for Polymer Research, Mainz, Germany

"Kinetic Growth Model of Carbon Nanotubes," A. Maiti, North Carolina State University, Raleigh, N.C.

"Scanning Tunneling Microscopy Studies of Thermodynamics of Strained Ge Epitaxial Overlayer on Si (001)," F. Wu, University of Wisconsin, Madison, Wis.

"Solid State Sensors for Combustion Control," L. Younkman, Ohio State University, Columbus, Ohio

"Dynamics and Structure of Confined Polymers by Neutron Small-Angle Scattering and Reflectometry," D. Perahia, Exxon Research and Engineering Co., Annandale, N.J.

"Self-Assembling Electron-Transport Chains at Electrodes Modified with Clay and Related Microporous Solids," D. Rong, California Institute of Technology, Pasadena, Calif.

[1]"Carbon Aerogels: An Overview of Structure-Property Relations," G. A. M. Reynolds, Massachusetts Institute of Technology, Cambridge, Mass.

"Numerical Simulations and Analytical Modeling of Semiconductor Quantum Wires," Y. Sun, Simon Fraser University, Barnaby, Canada

"Interlayer Coupling in Magnetic Multilayer Structures," Z. P. Shi, University of California-Davis, Davis, Calif.

"The Influence of Anisotropy and Pinning Effects on the Vortex Lattice: A Study Using the Decoration Technique," L. Gurevich, Physique de L'etat Condense, Saclay, France

"Understanding and Controlling Transient-Enhanced Dopant Diffusion in Silicon," P. A. Stolk, Lucent Technologies, Bell Laboratories, Murray Hill, N.J.

"Ag Monolayer Growth and Structure on Ni and Cu Surfaces," P. T. Sprunger, University of Aarhus, Aarhus, Denmark

"Resonant Ultrasound Spectroscopy Determination of the Complete Elastic Moduli of $La_{2-x}Sr_xCuO_4$," J. Sarrao, National High-Magnetic Field Laboratory, Tallahassee, Fla.

"Transmission Electron Microscopy of High-T_c Oxide Thin Films," E. J. Williams, IBM Research Division, Zürich, Switzerland

"Atomistic Studies of Ceramic-Metal Interfaces," D. N. Seidman, Northwestern University, Evanston, Ill.

"Materials for Lithium Ion Batteries," G. Ehrlich, University of Nantes, Nantes, France

"Self-Organizing Surface Structures in Strained-Layer Growth," J. D. Tersoff, IBM T. J. Watson Research Center, Yorktown Heights, N.Y.

"Casmir Forces Between Quantum Wells," B. E. Sernelius, Linköping University, Linköping, Sweden

"Atomistic Simulation of Grain Boundary Phenomena in Cu," M. Nomura, University of Illinois, Urbana, Ill.

"Development of Atomistic Potentials with Applications to Grain Boundary Segregation and Diffusion," J. B. Adams, University of Illinois, Urbana, Ill.

"*Ab Initio* Multiconfigurational SCF Calculations of Impurities and Defects in Calcium Flouride," A. C. Lewandowski, Naval Surface Warfare Center, Silver Springs, Md.

"Long-Range Phase Coherence in Proximity Coupled with Josephenson Junction Arrays," F. Hui, Ohio State University, Columbus, Ohio

"Fermi Edge Singularities in Nonlinear Absorption Spectra: Excitonic Polarons," I. Perakis, Vanderbilt University, Nashville, Tenn.

"Gettering of Metal Impurities in Silicon," D. Eaglesham, Lucent Technologies, Bell Laboratories, Murray Hill, N.J.

"Ion Implantation of Diamond and Diamond Films: Fundamentals and Applications," S. Prawer, University of Melbourne, Parksville, Australia

"X-Ray Diffraction and Electron Microscopy Studies on the Atomic Structure of Grain Boundaries in Metals and Ceramics," I. Majid, Massachusetts Institute of Technology, Cambridge, Mass.

"Do We Really Understand Low-Temperature Superconductors?" J. Freericks, Georgetown University, Washington, D.C.

"Ablation in the Appalachians: Challenges and Opportunities in Semiconductor Growth and Doping," C. M. Rouleau, ORNL/Oak Ridge Institute for Science and Education

"A Model System for Magnetic Multilayers: Pt-Co Surface Alloys on the Pt(111) Surface Studies with X-Ray Diffraction," V. Jahns, ORNL/Oak Ridge Institute for Science and Education

"Grain Boundaries in High-T_c Superconductors: Fundamental Aspects and Applications," J. Mannhart, IBM Research Laboratory, Zürich, Switzerland

"Impurity Gettering in Oxygen Precipitation at MeV Ion Implantation-Induced Defects in Silicon," A. Agarwal, North Carolina State University, Raleigh, N.C.

"Analysis of Damage Formation and Structural Evolution in Semiconductors and Metallic Thin Films," D. Maroudas, University of California, Santa Barbara, Calif.

"Shaking the Truth Out of Superconductors: Nonlinear and Chaotic Response of Quantized Magnetic Vortices in $NbSe_2$," L. DeLong, University of Kentucky, Lexington, Ky.

"Growth Exponents in the Dynamics of Phase Separation in Binary Fluids," G. Martinez-Piño, Federal University of Rio Grande de Sul, Porto Alegre, Brazil

"Thermoelectric Flux in a Bimetallic Superconducting Ring," C. Marinescu, Purdue University, Lafayette, Ind.

"Calculating ELNES From First Principles," C. J. Pickard, Cavendish Laboratory, Cambridge, United Kingdom

"Waves on a Metal Surface and Quantum Corrals," M. F. Crommie, Boston University, Boston, Mass.

"Quantum Monte Carlo Simulations of Electrons in Real Materials," R. M. Martin, University of Illinois, Champaign, Ill.

"Beyond the Quantum Hall Effect: Topological Considerations and Quantum Engineering," Q. Niu, University of Texas, Austin, Tex.

"Clean Thoughts About Dirty Superconductors," A. W. Overhauser, Purdue University, West Lafayette, Ind.

"Magnetic Quantum Well States: The Concept and the Implications to GMR Multilayers," D. Li, Argonne National Laboratory, Argonne, Ill.

"Low-Energy Excitations in an Incipient Antiferromagnet," J. J. Diesz, Georgetown University, Washington, D.C.

"Retarded Effective Potential in Time-Dependent Density Functional Theory," G. Vignale, University of Missouri, Columbia, Mo.

"Kinetics of Pt(111) Surfaces at Low Temperatures," M. Hohage, Forschungazentrum, Jülich, Germany

"Effect of Silver on Processing and Properties of Bi- and Ti-Based HTSC Materials," C. Park, Alfred University, Alfred, N.Y.

"Spin-Polarized Electron Scattering and Spin Dynamics of Ultrathin Magnetic Films," M. Plihal, Rutgers University, Piscataway, N.J.

"Dynamical X-Ray Scattering Near Critical Boundary Geometries: Synchrotron and Theoretical Studies," M. Baysal, Temple University, Philadelphia, Pa.

"Growing Atomically Flat Silver Film on GaAs," C.-K. Shih, University of Texas, Austin, Tex.

"Electron Density and Bonding in Crystals Studied by X-Ray and Neutron Diffraction," R. P. Ozerov, Mendeleev University of Chemical Technology, Moscow, Russia

"The Implantation and Annealing Effects of Yttrium Ion Implantation into Alumina," E. M. Hunt, Georgia Institute of Technology, Atlanta, Ga.

"Composite Fermion Description of Fractional Quantum Hall Systems," J. J. Quinn, The University of Tennessee, Knoxville, Tenn.

"Influence of Machining Forces on the Subsurface Damage of High-Strength Silicon Nitride," R. Ott, University of Alabama, Birmingham, Al.

"Electron-Irradiation-Induced Nucleation and Growth in Amorphous Ceramics," A. Meldrum, University of New Mexico, Albuquerque, N.M.

"Designer Molecules at Surfaces: Toys and Tools on Their Way to Nanotechnology," T. Jung, IBM Zürich Research Laboratory, Zürich, Switzerland

"Morphological Stability of the Solid-Liquid Interface During Rapid Solidification of Silicon-Tin," D. Hoglund, Eaton Corporation, Beverly, Mass.

[2]"Bond Effects on Ion Surface Charge Exchange," R. Souda, National Institute for Research in Inorganic Materials, Ibaraki, Japan

"Correlation of Bulk and Surface Phase Transitions in Complex Materials," J. Zhang, The University of Tennesee, Knoxville, Tenn.

[1]"Micro-Modeling of Aluminum Fabrication: Status and Research Issues," R. Shuey, ALCOA, Pittsburgh, Pa.

"The Physics and Chemistry of Silicon Interfaces: Hydrophilic Wafer Bonding and Si Layer Exfoliation," M. Weldon, Lucent Technologies, Bell Laboratories, Murray Hill, N.J.

"A New Type of Spin Glass in Spin Density Wave CrMn Alloys," V. Galkine, Federal University of Parana, Curitiba, Brazil

"Thickness-Dependent Magnetic Microstructures in Ultrathin Films: Co/Au(111)," H. Oepen, Max-Planck-Institut for Microstructural Physics, Halle, Germany

"Quantum Confinement Effects in Carbon Nanotubes," K. R. Subbaswamy, University of Kentucky, Lexington, Ky.

"Double Gap in the Spin-Peierls Compounds $CuGeO_3$," M. Ain, Comisseriat Energie Atomique, Saclay, France

"SPIX: A New Technique for Near-Surface Impurity Using PIXE," W. Lennard, University of Western Ontario, London, Ontario

"Magnetic Anisotropy in 2D Systems," Z. Qiu, University of California, Berkeley, Calif.

"Recent Developments in Coatings of Diamond and Other Hard Minerals," B. Stritzker, University of Augsburg, Augsburg, Germany

"Manifestation of the Quantum-Size Effect in Metallic Films," M. Jalochowski, University of M. Curie-Sklodowska, Lublin, Poland

"First-Principles Determination of the Effects of Impurities on Iron Grain-Boundary Cohesion," L. Zhong, Northwestern University, Evanston, Ill.

"Pulsed-Laser Deposition of Nanocrystalline Silicon Quantum Dots and Device Applications," T. Yashida, Matshushita Research Institute, Tokyo, Japan

"Ion Beam Analysis of Oxide Thin Films," M. Watamori, Osaka University, Osaka, Japan

"Growth Phenomena on Semiconductor Surfaces: From Atomic Diffusion to Formation of Nanostructures," E. Kaxiras, Harvard University, Cambridge, Mass.

"Superconducting Nonlocality as Seen in Low-Temperature Magnetization and Vortex Lattices," V. Kogan, Iowa State University, Ames, Iowa

"High-Resolution Synchrotron Radiation Core-Level Spectroscopy of Bare and C60-Covered Si(111) ($\sqrt{3} \times \sqrt{3}$) R30°-Ag Interfaces," G. Lay, Université de Provence, Marseille, France

"Mapping of Redox Energies of Materials for Lithium Batteries," A. Padhi, University of Texas, Austin, Tex.

"Step Energetics and Diffusion Barriers on Silicon (111)," S. Kodiyalam, University of Maryland, College Park, Md.

"Tape Casting of Ceramic Materials," T. Suwannasiri, Rutgers University, Piscataway, N.J.

"Supersonic Molecular Beams as a Tool in Establishing the Micro-Meso Connection in Energetic Thin-Film Deposition Processes," J. E. Engstrom, Cornell University, Ithaca, N.Y.

"Geometrical Influence on Collective Excitations," S. P. Apell, Chalmers University of Technology, Göteborg, Sweden

"Surface-Induced Phenomena at Pd (110) and PdAg Alloy," C. Hwang, Korea Research Institute of Standards and Science, Taejon, Korea

"Theory of Colossal Magnetoresistive Oxides," J. Zang, Los Alamos National Laboratory, Los Alamos, N.M.

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[1]Joint Solid State and Metals and Ceramics divisions seminar.

[2]Joint Chemical and Analytical Sciences and Solid State divisions seminar.

LUNCHEON SEMINARS

"Semiconductor Nanocrystals: Formation, Processing, and Optical Properties," J. Zhu, ORNL/Oak Ridge Institute for Science and Education

"Novel Transport Behavior in the Dissipative Regime of Superconductors," M. Kunchur, ORNL/Oak Ridge Institute for Science and Education

"Fast Diagnostics of the Pulsed-Laser Ablation Process," D. B. Geohegan, Solid State Division, ORNL

"Funny Interfaces...Fascinating Properties," H. H. Weitering, UT/ORNL Distinguished Scientist Program

"How to Use Nuclear Reactors to Clean Up the Environment," G. D. Wignall, Solid State Division, ORNL

"Melting in Two-Dimensional Lennard-Jones Systems," K. Chen, ORNL/Oak Ridge Institute for Science and Education

"Optical Reflection Diagnostics for Thin-Film Growth or How Thick is My Film?" G. E. Jellison, Jr., Solid State Division, ORNL

"Chemical Vapor Deposition from Molecular Jets," D. C. Lubben, Solid State Division, ORNL

"Unique Views of Materials Using a 300-kV STEM," P. D. Nellist, ORNL/Oak Ridge Institute for Science and Education

"From Here to Infinity and Back: Investigations on the Parent High-Temperature Superconductor $SrCuO_2$ Structural Derivatives," R. Feenstra, Solid State Division, ORNL

"Optical Switching of VO_2 Precipitates Embedded in Sapphire," L. Gea, ORNL/ORISE Postdoctoral Research Associate

"A Novel Mechanism for Cluster Diffusion and Dissociation on Metal (001) Surfaces," Z.-P. Shi, ORNL/Oak Ridge Institute for Science and Education

"Rocking Curves and Rolling Chambers: Surface Structure by X-Ray Diffraction," A. P. Baddorf, Solid State Division, ORNL

"Filling Submicron Features with Cu from a High Density Plasma," F. C. Doughty, ORNL/Oak Ridge Institute for Science and Education

"Superconducting Wire From the Home Depot: Will It Happen Soon?" D. P. Norton, Solid State Division, ORNL

"Coupled Spin and Charge Density Waves in Cr Alloys," R. S. Fishman, Solid State Division, ORNL

"Equilibrium Crystal Structure of $YBa_2Cu_3O_{7-x}$," B. C. Chaokoumakos, Solid State Division, ORNL

"Phonon Heterostructure Transport," P. Hyldgaard, The University of Tennessee, Knoxville, Tenn.

"Instability and Metastability During Strained-Layer Epitaxy," D. E. Jesson, Solid State Division, ORNL

"Pathways to Dissociation: What's the Deal?" A. T. Hanbicki, The University of Tennessee, Knoxville, Tenn.

"Effects of a Solid/Liquid Interface on a Complex Fluid Under Flow," P. D. Butler, ORNL/Oak Ridge Institute for Science and Education

"The Silicon Revolution and Its Materials Limits," L. C. Feldman, Vanderbilt University, Nashville, Tenn.

"Dopant Segregation at Semiconductor Grain Boundaries Through Cooperative Chemical Rebonding," A. Maiti, ORNL/Oak Ridge Institute for Science and Education

"Physics of Reengineering," J. F. Cooke, Solid State Division, ORNL

"Excitations in Free and Coupled Quantum Magnetic Dimers," D. A. Tennant, ORNL/Oak Ridge Institute for Science and Education

"Two Be or Not to Be? Beryllium—Bulk and Surface, Do They Have Anything in Common?" K. Pohl, The University of Tennessee, Knoxville, Tenn.

"Magnetic Dynamics in $YBa_2Cu_3O_{7-x}$," P. Dai, Solid State Division, ORNL

"Low-Energy Ion Implantation in Silicon Technology: Will Ion Implantation Still be Used in 2010?" A. Agarwal, ORNL/Oak Ridge Institute for Science and Education

SURFACE PHYSICS SEMINARS AND JOURNAL CLUB

"The Use of Optical Reflectance Anisotropy to Study Surface Electronic States, P. Hofmann, The University of Tennessee, Knoxville, Tenn.

"Pb-Induced Reconstructions on Ge(111)," J. Carpinelli, University of Pennsylvania, Philadelphia, Pa.

"H-Enhanced Diffusion on Be(0001)," R. Stumpf, Sandia National Laboratories, Albuquerque, N.M.

"The Local Structure of Adsorbed Atoms and Molecules as Determined by Photoelectron Diffraction," P. Hofmann, The University of Tennessee, Knoxville, Tenn.

"Coherent X-Ray Scattering," A. Baddorf, Solid State Division, ORNL

"Hydrodesulfurization of Thiophenes on Single-Crystal Metal Surfaces: Part II," D. Huntley, Chemical and Analytical Sciences Division, ORNL

"Science of the PEC '95," A. Hanbicki, University of Pennsylvania, Philadelphia, Pa.; P. Hofmann, The University of Tennessee, Knoxville, Tenn.; and C. Walters, University of Pennsylvania, Philadelphia, Pa.

"An Informal Discussion About Metal-Semiconductor Interfaces," F. Flores, Universidad Autonoma de Madrid, Madrid, Spain

"Electron-Electron Scattering in Far-Infrared Quantum Cascade Lasers," P. Hyldgaard, UT/ORNL Distinguished Scientist Program

"Sulfur Chemistry on Bimetallic Surfaces: Methanethiol on Ni-Covered W(001)," D. Mullins, Chemical and Analytical Sciences Division, ORNL

"The Use of Nonlinear Optics to Probe Surface Magnetism," C. Ying, Health Sciences Research Division, ORNL

"A Simple Model for Photoemission Peak Widths," B. E. Sernelius, Linköping University, Linköping, Sweden

"Ordered Surface-Alloy Phases Between Copper Single-Crystal Planes and Lithium," H. Tochihara, Hokkaido University, Hokkaido, Japan

"X-Ray Surface Scattering," S. E. Nagler, Solid State Division, ORNL; W. A. Hamilton, Solid State Division, ORNL; and J. L. Robertson, ORNL/Oak Ridge Institute of Science and Technology

"Enhanced Curie Temperature at the Surface of Gd(0001)," P. Dowben, University of Nebraska, Lincoln, Neb.

"Electronic Structure Calculations of Simple Metal Surfaces," E. Chulkov, Russian Academy of Sciences, Tomsk, Russia

"Theory of Magnetism/Multilayers and Surfaces," Z.-P. Shi, ORNL/Oak Ridge Institute of Science and Technology

"Advantages and Deficiencies of LDA Total Energy Calculations," R. Stumpf, Sandia National Laboratories, Albuquerque, N.M.

"*Ab Initio* Theory of Magnetic Response for Itinerant Systems: Bulk and Thin Films," A. Eguiluz, The University of Tennessee, Knoxville, Tenn.

"Shot Noise in an STM-Coulomb-Blockage System," P. Hyldgaard, UT/ORNL Distinguished Scientist Program

"A Tutorial (Uniformed) Discussion of Many-Body Effects at Surfaces," E. W. Plummer, UT/ORNL Distinguished Scientist

"Charge Density Waves: From Overhauser to Tosatti," J. M. Carpinelli, The University of Tennessee, Knoxville, Tenn.

"The Past, Present, and Future of Inelastic Electron Scattering," L. Kesmodel, Indiana University, Bloomington, Ind.

"Spin and Charge Density Waves: Can't We All Just Get Along?" R. S. Fishman, Solid State Division, ORNL

"Magnetic Properties in a Two-Dimensional Hubbard Model," Z. Shi, ORNL/Oak Ridge Institute of Science and Technology

"The Rotating, Jumping, Kicking, and Screaming of a Si Ad-Dimer on Si(100)" or "The RJKS Model of the Si Dimer," Z. Zhang, Solid State Division, ORNL

"My Research Interests: What Am I Doing? Where Am I Going? How Can Interface with ORNL?" E. W. Plummer, UT/ORNL Distinguished Scientist

"Trillions of X-Ray Photons Later: The Sn/Ge(111) CDW Revisited," A. P. Baddorf, Solid State Division, ORNL

"Friedel Oscillations in Two Dimensions," P. Hofmann, The University of Tennessee, Knoxville, Tenn.

HIGH-T_C SUPERCONDUCTIVITY SEMINARS

"Synthesis, Structure, and Superconductivity of $Ag_xHgBa_2CuO_{4+\delta}$ Compounds," H. Khan, FEM, Schwabish, Germany

"Recent High-T_c Superconductor Research at the Electro Technical Laboratory: Vortex-Glass Transitions, etc.," H. Yamasaki, Electro Technical Laboratory, Tsukuba, Japan

"Superconducting Nonlocality as Seen in Low-Temperature Magnetization and Vortex Lattices," V. Kogan, Iowa State University, Ames, Iowa

LECTURES AND SEMINARS BY DIVISION MEMBERS

M. Agamalian—National Institute of Standards and Technology, Gaithersburg, Maryland, "ORNL Double-Crystal Ultra Small-Angle Neutron Scattering Facility"; Brookhaven National Laboratory, Upton, New York, "Development of the Bonse-Hart Technique for Ultra Small-Angle Neutron Scattering and Neutron Optics"

A. P. Baddorf—Rutgers University, Piscataway, New Jersey, "Rocking Curves and Rolling Chambers: Surface Structure by X-Ray Diffraction"; Brookhaven National Laboratory, Upton, New York, "Thermal Contraction of the Cu(001) Surface"

J. B. Bates—Argonne National Laboratory, Argonne, Illinois, "Thin-Film Lithium Batteries"

L. A. Boatner—Oak Ridge National Laboratory Science and Engineering Research Semester Program, Oak Ridge, Tennessee, "The Growth and Application of Single Crystals"; The University of Tennessee Science Alliance Seminar, Knoxville, Tennessee, "The Growth and Characterization of Rare-Earth Orthophosphates"; Florida State University, Tallahassee, Florida, "The Physics of Welding"

P. D. Butler—National Institute of Standards and Technology, Gaithersburg, Maryland, "Reflection Geometry SANS"

B. C. Chakoumakos—Japan Atomic Energy Research Institute, Tsukuba, Japan, "Crystal Structure Systematics of the Cuprate Superconductors"

M. F. Chisholm—Lehigh University, Allentown, Pennsylvania, "Atomic Structure of Extended Defects in Semiconductors"

D. K. Christen—Michigan State University, East Lansing, Michigan, "Current Problems in High-Temperature Superconductors: Prospects for Improved Conductors"

A. G. Eguiluz—Universität Würzburg, Würzburg, Germany, "Self-Energies at Metal Surfaces"; Fritz-Haber-Institut der Max-Planck-Gesselschaft, Berlin, Germany, and Technical University of Dresden, Dresden, Germany, "*Ab Initio* Evaluation of Dynamical Electronic Response in Metals and its Comparison with Experiment"

J. A. Fernandez-Baca—Southern Illinois University, Carbondale, Illinois, "Neutron Scattering Studies of Magnetic Excitations in Solids"

R. S. Fishman—Oak Ridge National Laboratory, Oak Ridge, Tennessee, "Phase Diagram of Cr Alloys"; University of Missouri, Columbia, Missouri, University of Manitoba, Manitoba, Canada, and North Dakota State University, Fargo, North Dakota, "Spin Dynamics of Incommensurate Chromium Alloys"; Universidade de San Carlos, San Carlos, Brazil, Centro Barsileiro de Pesquisas Fisicas, Rio Brazil, and Universidade Federal Fluminense, Niteroi, Brazil, "Competition Between Interfacial Coupling and Spin-Density Wave Magnetism in Fe/Cr Multilayers and Wedges"

L. A. Gea—Arizona State University, Tempe, Arizona, "Optical Switching of Embedded Vanadium Dioxide Nanocrystals"

T. E. Haynes—Arizona State University, Tempe, Arizona, and Erato-Tanaka Solid Junction Project, Yokohama, Japan, "Solid-Phase Epitaxial Crystallization in Si: What Happens When We Add Ge and/or C?"; Motorola, Inc., Tempe, Arizona, "Ion Implantation and Recrystallization in SiGe Alloys and Heterostructures"; University of North Carolina, Chapel Hill, North Carolina, "Solid-Phase Epitaxial Crystallation in Si and SiGe Alloys"; University of Tokyo, Tokyo, Japan, "Solid-Phase Epitaxial Crystallization in Si-Based Alloys and Some Ceramic Thin Films"; Asahi Glass Research Center, Yokohama, Japan, "Recent Progress in Ion Implantation Research"

O. W. Holland—Brookhaven National Laboratory, Upton, New York, "The Synthesis of SOI by High-Dose O^+-Implantation: A Vehicle for Providing New Understanding of the Ion-Solid Interaction"; Lucent Technologies, Murray Hill, New Jersey, "The Effects of Ion-Induced Damage on Implantation Processing of Semiconductors"

G. E. Jellison, Jr.—Pennsylvania State University, University Park, Pennsylvania, "Optical Functions of Transparent Materials Determined Using Spectroscopic Ellipsometry"

D. E. Jesson—University of Alabama, Birmingham, Alabama, "How Semiconductors Grow"; University of Oxford, Oxford, United Kingdom, "New Insights into Quantum Dots"

M. N. Kunchur—Cornell University, Ithaca, New York, and Clemson University, Clemson, South Carolina, "Novel Phenomena in Superconductivity Observed at Extreme Dissipation Levels"

J. S. Lin—National Tsing-Hua University, Hsin-chu, Taiwan, "Principles and Applications of Small-Angle X-Ray and Neutron Scattering"

D. H. Lowndes—University of Missouri, Columbia, Missouri, "Pulsed-Laser Ablation Growth and Doping of Epitaxial Compound Semiconductor Films"; University of Tsukuba, Tsukuba, Japan, Nippon Steel Central Research Laboratory, Kawasaki, Japan, Tokyo Institute of Technology, Yokohama, Japan, Kobe Steel Research Laboratory, Seishin, Japan, and Matsushita Central Research Laboratory, Kyoto, Japan, "Growth and *p*-Type Doping of ZnTe by Pulsed-Laser Ablation"

D. C. Marinescu—Vanderbilt University, Nashville, Tennessee, "Thermoelectric Flux in Bimetallic Superconducting Rings"

S. E. Nagler—University of California at Los Angeles, Los Angeles, California, "Neutron Scattering and Magnetic Materials"

P. D. Nellist—Northwestern University, Evanston, Illinois, "Unique Views of Materials: Atomic Resolution Z-Contrast Imaging"

S. J. Pennycook—McMaster University, Hamilton, Ontario, Canada, "Toward Atomic Resolution Microanalysis"; Case Western Reserve University, Cleveland, Ohio, "New Insights into Materials Through Z-Contrast STEM"; North Carolina State University, Raleigh, North Carolina, "Toward the Atomic Level Engineering of Grain Boundaries in Ceramic Superconductors"

K. Pohl—Sandia National Laboratories, Livermore, California, and Brookhaven National Laboratory, Upton, New York, "Surface Structure: Do We Really Understand What is Going on? A Case Study of Beryllium Surfaces"

D. B. Poker—Pacific Northwest National Laboratory, Richland, Washington, "Ion Beams in Fundamental and Applied Physics"

J. J. Quinn—Michigan State University, East Lansing, Michigan, and Oak Ridge National Laboratory, Oak Ridge, Tennessee, "Composite Fermion Excitations and the Energy Spectra of Quantum Hall Systems"; University of South Carolina, Columbia, South Carolina, "Composite Fermions and the Fractional Quantum Hall Effect"; Department of Energy, Germantown, Maryland, "Composite Fermions Description of Quantum Hall Systems"; University of California at Santa Barbara, Santa Barbara, California, "Fermi Liquid Shell Model of Composite Fermions in Quantum Hall Systems"; University of Pennsylvania, Philadelphia, Pennsylvania, "Fermi Liquid Shell Model Approach to Composite Fermion Picture of Fractional Quantum Hall Systems"; Oak Ridge National Laboratory, Oak Ridge, Tennessee, "Fermi Liquid Shell Model of Composite Fermions in Quantum Hall Systems"; The University of Tennessee, Knoxville, Tennessee, "The Composite Fermion Hierarchy"; National Research Council of Canada, Ottawa, Canada, "Composite Fermions and the Hierarchy of Fractional Quantum Hall States"; State University of New York, Buffalo, New York, "Composite Fermions and the Photoluminescence Spectrum of Quantum Hall Systems"; State University of New York, Buffalo, New York, "The Composite Fermion Hierarchy of Fractional Quantum Hall States"

A. K. Swan—Arizona State University, Tempe, Arizona, "Flux Dependence in the Submonolayer Growth Kinetics of Cu on Cu(100)"

J. R. Thompson—Polytechnico di Torino, Torino, Italy, "Processing High-Temperature Superconductors for Enhanced Current Conduction"; Bar Ilan University, Bar Ilan, Israel, "Comparative Study of the Characteristic Length Scales and Fields of Hg-Based High-T_c Superconductors"; Forschungszentrum Karlsruhe, Germany, and Imperial College, London, United Kingdom, "The Impact of Tailored Defects on Length Scales and Current Conduction in High-T_c Superconductors"; Research Institute for Noble Metals and Metal Chemistry, Schwaebisch-Gmuend, Germany, "Nanocomposites with Ni and Co Particles: Synthesis and Magnetic Properties"

J. F. Wendelken—Royal Institute of Technology, Stockholm, Sweden, University of Aarhus, Aarhus, Denmark, Max Planck Institut für Microstructural Physics, Halle, Germany, and IBM Zurich Research Laboratory, Rüschlikon, Switzerland, "Epitaxial Growth and Energy Barriers: Cu/Cu(100)"

C. W. White—Ritumeikan University, Kyoto, Japan, and Kyoto University, Kyoto, Japan, "Research Activities in the Surface Modification and Characterization Research Center at ORNL"

G. D. Wignall—University of North Carolina, Chapel Hill, North Carolina, "Neutron Scattering Characterization of Polymerization Mechanisms in Supercritical Carbon Dioxide"; Imperial Chemical Industries, Wilton, United Kingdom, "Small-Angle Scattering Studies of Synthetic Polymers"; Reactor Radiation Division Seminar, Oak Ridge National Laboratory, "Small- and Ultra Small-Angle Neutron Scattering Studies of Miscibility and Segregation in Blends of Linear and Branched Polyethylenes"

Z. Zhang—Arizona State University, Tempe, Arizona, "Atomic-Scale Manipulation of Growth Kinetics in Nucleation and Growth"; Hong Kong University, Hong Kong, "Microscopic Mechanisms of Two-Dimensional Pattern Formation and Thin-Film Epitaxy"; Fritz-Haber Institut der MPG, Berlin, Germany, "Microscopic Mechanisms of Two-Dimensional Pattern Formation and Thin-Film Epitaxy"; University of Twente, Twente, the Netherlands, "Rate Manipulation in Homoepitaxy"; University of Ulm, Ulm, Germany, "Point Defects on Si(001): Their Energetics, Dynamics, and Roles in Thin-Film Growth"; Technical University of Denmark, Lyngby, Denmark, and Forschungszentrum, Jülich, Germany, "Microscopic Mechanisms of 2D Pattern Formation"; Lehigh University, Bethlehem, Pennsylvania, and Emory University, Atlanta, Georgia, "Microscopic Mechanisms of 2D Pattern Formation and Thin-Film Epitaxy"; University of Nevada at Las Vegas, Las Vegas, Nevada "Microscopic Mechanisms of 2D Pattern Formation at Surfaces"; University of California at Davis, Davis, California, "Atomistic Aspects of 2D Pattern Formation and Thin-Film Epitaxy"; University of California at Davis, Davis, California, and University of Texas at Austin, Austin, Texas, "Dynamics of Ad-Dimers at Surfaces"; University of California at Santa Barbara, Santa Barbara, California, "Electronic Growth of Metallic Overlayers on Semiconductor Substrates"

Scientific Activities, Awards, & Honors

A. P. Baddorf	Treasurer, Tennessee Valley Chapter of the American Vacuum Society, 1995–1996 Executive Board, Complex Materials Consortium CAT, 1995–present
J. B. Bates	Member, Technology Working Group on Energy Storage Systems, National Electronic Manufacturing Initiative (NEMI), 1995–present Editor, *Thin-Film Solid Ionic Devices and Materials*, The Electrochemical Society, Inc., Pennington, New Jersey, 1996 Lockheed Martin Energy Research Corporation, Inventor of the Year, 1996 R&D 100 Award for "Thin-Film Rechargeable Lithium Batteries," 1996
L. A. Boatner	Chairman, ORNL Alvin M. Weinberg Lectureship Selection Committee Elegant Work Prize of the Institute of Materials, United Kingdom, 1997 Federal Laboratory Consortium Award for Excellence in Technology Transfer, 1997 R&D 100 Award for "Potassium Tantalate (Niobate) Substrate," 1996 Lockheed Martin Energy Research Technical Achievement Award, 1997 Best Poster Paper Award, Fourth International Conference on Trends in Welding Research, Gatlinburg, Tennessee, 1995 First in Class Award, ASM International/International Metallographic Society Competition, 1995. Reviews Editor, *Journal of Materials Research*, 1995–present Member, Committee on International Scientific Affairs of the American Physical Society, 1996–1997 Member, NASA Microgravity Science and Applications Division, Review Panel on Electronic Materials, 1995. Member, Optical Society of America/Materials Research Society Congressional Science and Engineering Fellowship Selection Committee, 1995 Member, NASA Science Working Group for the Space Station Furnace Facility, International Space Station Alpha, 1995–1997 Research Advisor, DOE/GLCA/ACM Oak Ridge Science Semester 1995–1996 Associate Editor, *Optical Materials* Member, Executive Committee, American Association for Crystal Growth

Member, Vitality Committee of the Glass and Optical Materials Division, American Ceramic Society, 1995
Chairman, ORNL Corporate Fellows Council, 1997; Vice Chairman 1995–96
Member, International Advisory Board, 11th International Conference on Crystal Growth, 1993–1995
Member, William Hunt Eisenman Rare Book Committee of ASM International, 1996
Member, Awards, Academic Affairs, and External Affairs Committees, Materials Research Society, 1995–1996
Co-Editor, *Crystal Growth '95*, 1996
Session Chairman, Materials Research Society Symposium, Boston, Massachusetts, December 1995
Member, Ph.D. Thesis Committee, University of New Mexico, 1997
Session Chairman, 99th Annual Meeting of the American Ceramic Society, 1997
Chairman, ORNL-Universidad Nacional Autonoma de Mexico Joint Steering Committee 1993–1996
Thesis Advisor, ORNL Professional Internship Program, 1995–1996
Member, Advisory Committee, DOE-EPSCoR Program for Research in Puerto Rico

J. D. Budai

Participant, DOE Center of Excellence in Nanoscale Materials, 1994–1995
Lockheed Martin Energy Systems Significant Event Award, 1996
DOE Materials Sciences Research Competition Award for Significant Implication for DOE Related Technologies in Solid State Physics, 1996
Lockheed Martin Energy Research Technical Achievement Award, 1997
Lockheed Martin Energy Research Corporation NOVA Award, 1997

B. C. Chakoumakos

Correspondent for *Neutron News*, 1994–present
Member, Research Committee for the Institute for Solid State Physics, University of Tokyo–U.S. Department of Energy Cooperative Program on Neutron Scattering, 1995–present
Member, Research Committee for the Japan Atomic Energy Research Institute–U.S. Department of Energy Cooperative Program on Neutron Scattering, 1995–present
Research Advisor, ORNL/Science and Energy Research Semester Program, 1995
Member, Intense Pulsed Neutron Source/Manual Lujan Neutron Scattering Center Program Advisory Committee, 1996–present
Grand Awards Judge for Chemistry, International Science and Engineering Fair, Louisville, Kentucky, May 1997

D. K. Christen

Lockheed Martin Energy Research Corporation R&D Accomplishment Award, 1997
DOE Materials Sciences Research Competition Award for Significant Implications for Energy Related Technologies in Solid State Physics, 1996

	Lockheed Martin Energy Research Corporation Significant Event Award, 1996
	Co-Organizer, USAF-Sponsored Workshop on Flux, Quantum, and Mesoscopic Effects in Superconducting Materials and Devices, Santa Fe, New Mexico, August 1997
	Committee Member, NSF/ONR Workshop on Research Needs and Opportunities in Superconductivity, Monterey, CA, February 1997
	Co-Organizer, Joint MRS/ISTEC Workshop on Superconductivity, Maui, Hawaii, June 1997
	Technical Program Committee Member and Delegate, U.S.-Japan Workshop on High-T_c Superconductivity, Tsukuba, Japan, October 1995
	Session Chairman, CEC/ICMC Conference, Columbus, Ohio, July 1995
	Co-Organizer/Session Chairman, Joint MRS/ISTEC Workshop on Superconductivity, Maui, Hawaii, June 1995
	Member, Technical Advisory Committee, New York State Institute on Superconductivity, SUNY Buffalo, New York, June 1994–present
	Adjunct Professor, Department of Physics, The University of Tennessee, Knoxville, 1988–present
J. F. Cooke	Member, ORNL Fix-It Committee
	Member, Advisory Committee for Louisiana State University High Performance Computing Center
	Member, ORNL Steering Committee: SAP Implementation, 1997–present
	Programmatic Lead for Acquisition Core Team, Delta Project, 1997–present
N. J. Dudney	Associate Editor, *Journal of the American Ceramic Society*, 1986–present
	R&D 100 Award for "Thin-Film Rechargeable Lithium Batteries," 1996
R. Feenstra	R&D 100 Award for "Potassium Tantalate (Niobate) Substrates," 1996
	Federal Laboratory Consortium Award for Excellence in Technology Transfer, 1997
R. S. Fishman	Co-Chairman, International Conference of Condensed Matter Physics Workshop on Itinerant Magnetism, Brasilia, February 1997
D. B. Geohegan	Vice Chair, 1998 Gordon Conference on Laser Materials Interactions (Chair in 2000)
	Co-Chairman, Fourth International Conference on Laser Ablation (COLA'97), Monterey, California (to be held July 1997)
	Co-Chairman, Third International Conference on Laser Ablation (COLA'95), Strasbourg, France, May 1995

	Editorial Board, *Applied Physics Letters; Journal of Applied Physics*
	Co-Editor, *Proceedings of the Fourth International Conference on Laser Ablation*, Elsevier-North Holland, 1997
S. M. Gorbatkin	Co-Editor, *Thin Films and Surfaces for Bioactivity and Biomedical Applications*, Materials Research Society, Pittsburgh, Pennsylvania, 1996
W. A. Hamilton	Member, Elastic Scattering Working Group, Neutron Instrumentation for a Long-Pulse Spallation Source, Berkeley, California, April 1995
	Member, BESAC Subpanel on Spallation Source Upgrades, Washington, D.C., January 1996
	Member, Organizing Committee, Workshop on Methods of Neutron Scattering: Instrument Design, September 1996
	Organizer, Reflectometry Working Group, Users' Workshop on Instrumentation Needs and Performance Metrics for the Next Generation Spallation Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee, October 1996
T. E. Haynes	Member, Program Committee, Tenth International Conference on Ion Beam Modification of Materials, Albuquerque, New Mexico, September 1996
	Member, Technical Advisory Committee on Materials and Bulk Process Sciences, Semiconductor Research Corporation
	Member, International Organizing Committee, Symposium on Materials Synthesis and Modification by Ion and/or Laser Beams, 1996 Conference of Materials Research Society of Japan, Makuhari, Japan, May 1996
	Member, Organizing Committee, 1997 Conference on Surface Modification of Metals by Ion Beams, Gatlinburg, Tennessee (to be held September 1997)
	Research Visitor, Bell Laboratories/Lucent Technologies, Murray Hill, New Jersey, 1994–1997
	Adjunct Professor, Department of Chemical, Biology, and Materials Engineering, Arizona State University, Tempe, Arizona, 1995–present
	Adjunct Professor, Department of Physics, University of North Texas, Denton, Texas, 1996–present
G. E. Jellison, Jr.	Program Committee, Second International Conference On Spectroscopic Ellipsometry, Charleston, South Carolina (to be held in May 1997)
	Editorial Board, *Applied Physics Communications*, 1991–1995
D. E. Jesson	Editorial Board, *Micron*
	Co-Editor, *Evolution of Epitaxial Structure and Morphology*, Vol. 399 Materials Research Society, Pittsburgh, Pennsylvania, 1995

Co-Organizer, "Evolution of Epitaxial Structure and Morphology," Materials Research Society Fall Meeting, Boston, November 1995
Principal Organizer, "Structure and Morphology of Epitaxial Thin Films," TMS Annual Meeting, Anaheim, California, February 1996
Lockheed Martin Energy Research Publication Award, 1996
Session Chairman, Materials Research Society Fall Meeting, Boston, Massachusetts, November 1995
Session Chairman, TMS Annual Meeting, Anaheim, California, February 1996

H. R. Kerchner

Co-Organizer, Mini-Workshop on High-Temperature Superconductors at the National Educator's Workshop NEW: Update 95, Oak Ridge, Tennessee, November 1995

B. C. Larson

Chairman, Cornell High-Energy Synchrotron Source Policy and Advisory Board, 1994–1997
ORNL Project Leader, UNI-CAT Synchrotron Beam Line Construction Collaboration Project

D. H. Lowndes

Professor, The University of Tennessee, Knoxville, Tennessee
Member, Ph.D. Thesis Committees, The University of Tennessee
Co-Chairman, Symposium on Film Synthesis and Growth Using Energetic Beams, Spring Meeting of th Materials Research Society, San Francisco, California, April 1995
Session Chair, Materials Research Society, San Francisco, California, 1995
Member, International Organizing Committee, Third International Conference on Laser Ablation (COLA-95), Strasbourg, France, May 1995
Co-Chairman, Symposium on Advances in Laser Ablation of Materials, Spring Meeting of the Materials Research Society, San Francisco, California (to be held April 1998)
Member, Program Committee, Laser Applications in Microelectronic and Optoelectronic Manufacturing III, San Jose, California (to be held April 1998)
Member, International Organizing Committee, Fourth International Conference on Laser Ablation (COLA-97), Monterey, California (to be held July 1997)

D. C. Lubben

Organizer, Tennessee Valley Chapter, American Vacuum Society Exhibition, 1993–1997
Judge, Southern Appalachian Regional Science Fair, 1995–1997

C. F. Luck

R&D 100 Award for "Thin-Film Rechargeable Lithium Batteries," 1996

D. G. Mandrus

Lockheed Martin Energy Research Publication Award, 1997
Session Chairman, Spring Meeting of the Materials Research Society, San Francisco, California (to be held April 1997)

	Participant, Workshop on Instrumentation Needs and Performance Metrics for the National Spallation Neutron Source, Oak Ridge, Tennessee, October 1996
F. A. Modine	Member, Science and Technology Partnerships Reengineering Team, 1997 Co-Chairman, Guests and Users Process Reengineering Team, 1997 Chairman and Committee Member, ER-LTR Proposal Review Panel, 1996–1997 Division Chairman, United Way Campaign, 1996–1997
H. A. Mook	Chairman, International Conference on Neutron Scattering, Toronto, Canada, 1997
S. E. Nagler	Member, Executive Committee, Los Alamos Neutron Scattering Center Users' Group Member, Review Committees for Natural Sciences and Engineering and Interdisciplinary Science, Research Council of Canada, Chalk River Nuclear Laboratories, Chalk River, Canada Chair, Review Committee, DOE Scientific Facilities Initiatives Organizing Committee, Workshop on Instrumentation Needs and Performance Metrics for the National Spallation Neutron Source, Oak Ridge, Tennessee, October 1996 Program Committee, International Conference on Neutron Scattering '97, Toronto, Canada, 1997 Member, Brookhaven Advisory Committee for Neutron Scattering (Condensed Matter Physics) Adjunct Professor of Physics, University of Florida, Gainesville, Florida
D. P. Norton	Co-Editor, *Advanced Laser Processing of Materials—Fundamentals and Applications*, Vol. 397, Materials Research Society, Pittsburgh, Pennsylvania, 1995
D. B. Poker	Co-Chairman, Symposium on Ion-Solid Interactions for Materials Modification and Processing, Materials Research Society Fall Meeting, Boston, Massachusetts, 1995 Chairman, Materials Research Society Bound Volumes Subcommittee of the Publications Committee Member, Editorial Board, *Nuclear Instruments and Methods in Physics Research Section B* Co-Editor, *Ion Solid Interactions for Materials Modification and Processing*, Materials Research Society, Pittsburgh, Pennsylvania, 1996 Member, International Committee, Japan MRS Symposium N: Materials Synthesis and Modification by Ion Beams and/or Laser Beams, Chiba, Japan, 1996 Member, Materials Research Society Publication Committee Member, Organizing Committee, 10th International Conference on Surface Modification of Metals by Ion Beams, Gatlinburg, Tennessee, October 1997 Member, ORNL Seed Money Committee, 1995–1996

Member, Program Committee, 10th International Conference on Surface Modification of Materials, Albuquerque, New Mexico, 1996

Member, Organizing Committee, 1997 Conference on Surface Modification of Metals by Ion Beams, Gatlinburg, Tennessee (to be held September 1997)

Session Organizer, International Conference on the Application of Accelerators in Research and Industry, Denton, Texas, 1996

J. B. Roberto

ORNL Manager of the Year, Lockheed Martin Energy Research Corporation, 1997

Chair, Division of Materials Physics, American Physical Society (1997), Vice-Chair (1996)

Vice-Chair, Solid State Sciences Committee, National Research Council, 1995–1997

Vice-Chair, Committee on Condensed Matter and Materials Physics, National Research Council, 1996–present

Acting Associate Laboratory Director for Advanced Materials, Physical, and Neutron Sciences, ORNL, 1997

Member, ORNL Reengineering Steering Committee, 1996–present, Chair, 1996

Participant, Senior Assessment and Development Institute, Lockheed Martin Corporation, Maryland, June 1996

Member, Council on Materials Science and Engineering, Southeastern Universities Research Association, 1994–present

Member, Organizing Committee, "Driving Innovation Through Materials Research," Solid State Sciences Committee Forum, Washington, D.C., February 1996

Member, Organizing Committee, "Workshop on Condensed Matter and Materials Physics," National Research Council, Washington, D.C., July 1996

Co-Editor, "Driving Innovation Through Materials Research," *Proceedings of the Solid State Sciences Committe Forum*, National Research Council, September 1996

Co-Editor, "Instrumentation for a High-Power Pulsed Spallation Neutron Source," *Proceedings of the Workshop on Instrumentation Needs and Performance Metrics for the National Spallation Neutron Source*, 1997

Member, Organizing Committee, "Condensed Matter and Materials Physics: Into the Next Century," National Research Council Workshop, Washington, D.C. (to be held September 1997)

Member, Organizing Committee, March Meeting of the American Physical Society, Los Angeles, California (to be held in 1998)

Member, Organizing Committee, Forum of the Solid State Sciences Committee, Washington, D.C. (to be held in 1998)

Panelist, Forum on Condensed Matter and Materials Physics, Materials Research Society Fall Meeting, Boston, Massachusetts, December 1996; American Physical Society March Meeting, Kansas City, MO, March 1997

Focus Area Coordinator, DOE Center of Excellence in Synthesis and Processing, 1993–present

	Chair, Advisory Review Board, *Journal of Materials Research*, 1993--present
	Chair, Nominating, Fellowship, and Adler Award Committees, Division of Materials Physics, American Physical Society, 1997
	Member, Committee on Public Affairs, Materials Research Society, 1995--present
B. C. Sales	Editorial Advisory Board, *Journal of Physics and Chemistry of Solids*
	Lockheed Martin Energy Research Publication Award, 1997
	Lockheed Martin Energy Research Invention Award, 1997
A. K. Swan	Chair, Awards Committee, Tennessee Valley Chapter of the American Vacuum Society, September 1995–present
J. R. Thompson	Professor of Physics, The University of Tennessee, Knoxville, Tennessee
	Exceptional Service Award, Oak Ridge Centers for Manufacturing Technology, March 1997
	Co-Organizer, USAF-Sponsored Workshop on Flux, Quantum, and Mesoscopic Effects in Superconducting Materials and Devices, Santa Fe, New Mexico, August 1997
C. W. White	Member, External Affairs, Publications, and Long-Term Planning Committees of the Materials Research Society
	Editorial Board, *Journal of Material Chemistry and Physics*
	Member, Ion Beam Modification of Material International Committee
G. D. Wignall	Lockheed Martin Energy Research R&D Accomplishment Award, 1996
	DOE Materials Sciences Award for Outstanding Scientific Accomplishment, 1996
	Lockheed Martin Energy Research R&D Accomplishment Award, 1997
J. M. Williams	Chairman, 1997 Conference on Surface Modification of Metals by Ion Beams, Gatlinburg, Tennessee (to be held September 1997)
S. P. Withrow	Member, Organizing Committee, 1997 Conference on Surface Modification of Metals by Ion Beams, Gatlinburg, Tennessee (to be held September 1997)
Z. Zhang	Session Chair, 10th Annual Workshop on "Recent Developments in Computer Simulation Studies in Condensed Matter Physics," Athens, Georgia, February 1997
R. A. Zuhr	Exhibition Chairman, 1997 Conference on Surface Modification of Metals by Ion Beams, Gatlinburg, Tennessee (to be held September 1997)

Personnel Changes

New Staff Members

A. *Scientific Staff*

P. Dai, University of Missouri–Columbia, Columbia, Missouri
D. C. Marinescu, Purdue University, Evanston, Indiana
J. L. Robertson, University of Houston, Houston, Texas
C. M. Rouleau, University of Florida, Gainesville, Florida
M. Yoon, Massachusetts Institute of Technology, Cambridge, Massachusetts (10/6/97)
J. Zhang, Syracuse University, Syracuse, New York (9/2/97)

B. *Administrative and Technical Support Staff*

I. Dunbar, Technician (9/15/97)
J. A. Kolopus, Technician
S. A. Moore, Technician

C. *Leased Personnel*

S. R. Averell, Secretary
H. J. Dunlap, Secretary
C. D. Evans, Research Scientist
C. R. Hurley, Secretary
K. Nylander, Secretary

Staff Transfers and Terminations

A. *Scientific Staff*

S. M. Gorbatkin (voluntary resignation)
G. R. Gruzalski (transferred to Central Management Offices)
T. Kaplan (transferred to Computer Science and Mathematics Division)
C. E. Klabunde (retirement)
M. E. Mostoller (retirement)
M. T. Robinson (retirement)
J. M. Williams (retirement)

B. *Administrative and Technical Support Staff*

B. J. Copeland (retirement)
S. J. Cox (transferred to Benefit Plans Office)
T. C. Estes (retirement)

Guest Assignments

A. *Scientific Staff*

G. Aeppli,* NEC Research Institute, Inc., Princeton, New Jersey
J. W. Cable, Oak Ridge National Laboratory Retiree
G. S. Canwright, The University of Tennessee, Knoxville, Tennessee
H. R. Child, Oak Ridge National Laboratory Retiree
D. F. Chillura-Martino, University of Palermo, Palermo, Italy
H. L. Davis, Oak Ridge National Laboratory Retiree
A. Eguiliuz,† ORNL/UT Distinguished Scientist The University of Tennessee, Knoxville, Tennessee
L. C. Feldman,* Vanderbilt University, Nashville, Tennessee
J. A. Gaspar, Universidad de Sonora, Sonora, Mexico
L. J. Gillespie, Medtronics, Inc., Brooklyn Center, Minnesota
F. X. Hart, University of the South, Sewanee, Tennessee
M. Hubermann, Occidental College, Pasadena, California
N. H. Hur, Korean Research Institute of Standards and Science, Yusong, Korea
R. P. Joshi, Old Dominion University, Norfolk, Virginia
L. J. Magid, The University of Tennessee, Knoxville, Tennessee
G. D. Mahan,†† The University of Tennessee, Knoxville, Tennessee
G. G. Martinez-Pino, The University of Tennessee, Knoxville, Tennessee
R. M. Moon, Oak Ridge National Laboratory Retiree
Q. Niu, University of Texas at Austin, Austin, Texas
I. M. Obaidat, University of Illinois, Urbana, Illinois
M. Okada, University of Tokyo, Tokyo, Japan
J. Ossandon, University of Talca, Talca, Chile
S. T. Pantelides,* Vanderbilt University, Nashville, Tennessee
E. W. Plummer,†† The University of Tennessee, Knoxville, Tennessee
J. J. Quinn, The University of Tennessee, Knoxville, Tennessee
J. Rankin, Brown University, Providence, Rhode Island
B. E. Sernelius, Linkoping University, Linkoping, Sweden
M. Y. Shaikh, Atomic Energy Research Establishment, Bangladesh
H. G. Smith, Oak Ridge National Laboratory Retiree
J. O. Sofo, Universidad de Cuyo, Instituto Balseiro, Bariloche, Argentina
A. Triolo, University of Palermo, Palermo, Italy
R. Triolo, University of Palermo, Palermo, Italy
D. G. Wallis, University of Illinois–Chicago, Chicago, Illinois
R. D. Westbrook, Oak Ridge National Laboratory Retiree
H. H. Weitering, The University of Tennessee, Knoxville, Tennessee
M. K. Wilkinson, Oak Ridge National Laboratory Retiree
F. W. Young, Jr., Oak Ridge National Laboratory Retiree
J. L. Zarestky, Ames Laboratory/Iowa State University, Ames, Iowa
J. Zhang, The University of Tennessee, Knoxville, Tennessee

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*ORNL Distinguished Visiting Scientist
†ORNL/UT Collaborating Scientist
††ORNL/UT Distinguished Scientist

B. ***Postgraduate Research Participation Program***

M. M. Agamalian, State University of Tibilisi, Tibilisi, Russia
A. Agarwal, North Carolina State University, Raleigh, North Carolina
M. Bartiowiak, A. Michiewicz University, Poznan, Poland
P. D. Butler, The University of Tennessee, Knoxville, Tennessee
Keming Chen, Fudan University, Shanghai, China
Kun Chen, University of Georgia, Athens, Georgia
J. H. Cho, Pohang University of Science and Technology, Pohang, Korea
H.-M. Christen, Ecole Polytechnique Federale, Lausanne, Switzerland
P. Dai, University of Missouri, Columbia, Missouri
F. C. Doughty, University of Maryland, College Park, Maryland
G. Duscher, Max-Planck-Institut für Metallforschung, Stuttgart, Germany
L. Gavioli, Universita de Modena, Modena, Italy
L. Gea, Universite Claude Bernard, Lyon, France
M. J. Godbole, The University of Tennessee, Knoxville, Tennessee
G. Gvalani, Duke University, Durham, North Carolina
P. T. Hofmann, The University of Tennessee, Knoxville, Tennessee
Y. C. Hui, Ohio State University, Columbus, Ohio
P. A. Hyldgaard, The University of Tennessee, Knoxville, Tennessee
V. Jahns, University of München, München, Germany
K.-J. Jin, Chinese Academy of Science, Beijing, China
V. M. Keppens, Katholic Universitaet Leuven, Leuven, Belgium
M. N. Kunchur, Rutgers University, Piscataway, New Jersey
B. S. L. Kwak, Georgia Institute of Technology, Atlanta, Georgia
K. C. Lin, Michigan State University, East Lansing, Michigan
C. L. Liu, University of Illinois, Urbana, Illinois
A. Maiti, North Carolina State University, Raleigh, North Carolina
A. G. Malchoukov, USSR Academy of Sciences, Moscow, Russia
Y. B. Melnichenko, Institute of Macromolecular Chemistry, Kiev, Ukraine
P. D. Nellist, University of Cambridge, Cambridge, United Kingdom
B. J. Neudecker, University of Stuttgart, Stuttgart, Germany
W. W. Pai, University of Maryland, College Park, Maryland
C. Park, Alfred University, Alfred, New York
L. H. Peng, Harvard University, Cambridge, Massachusetts
C. S. Proteau, ISMRA–CRISMAT, Caen, France
A. A. Puretzky, Moscow Institute for Physics and Technology, Moscow, Russia
S. M. Quinlan, The University of Tennessee, Knoxville, Tennessee
J. L. Robertson, University of Houston, Houston, Texas
C. M. Rouleau, University of Florida, Gainesville, Florida
W. D. Schöne, Technical University of Berlin, Berlin, Germany
X. Shi, University of Rhode Island, Kingston, Rhode Isaland
Z. P. Shi, New York University, New York, New York
J. Sofo, Instituto Balseiro, Balseiro, Argentina
D. A. Tennant, University of Oxford, Oxford, United Kingdom
A. Ueda, Osaka City University, Osaka, Japan
V. S. Viswanath, University of Rhode Island, Kingston, Rhode Island
A. A. von Zomeren, Delft University, Delft, the Netherlands
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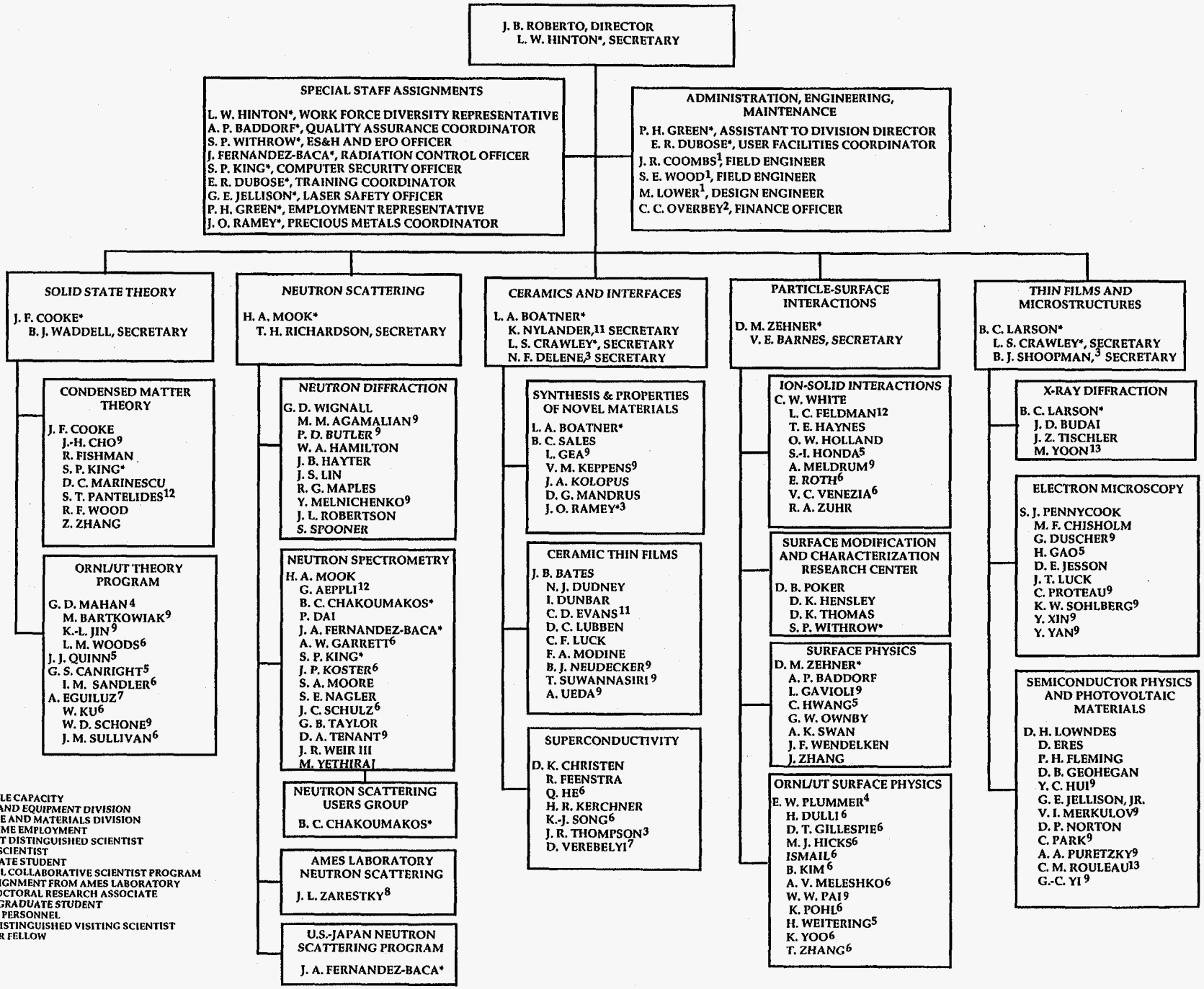

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