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CENTER FOR MATERIALS SCIENCE
LOS ALAMOS NATIONAL LABORATORY

STATUS REPORT
OCTOBER 1, 1990 THROUGH SEPTEMBER 30, 1991

Compiled by Don M. Parkin and A. M. Boring
October 1, 1991

Photograph by Chris J. Lindberg

Los Alamos
NATIONAL LABORATORY

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CONTENTS

	Page
CENTER DIRECTOR'S OVERVIEW	1
I. INTRODUCTION	4
II. CMS RESEARCH	7
Polycrystal Plasticity and Texture Development - Kocks	8
Metastable Phases and Microstructures - Schwarz	12
Interfaces and Other Defects in Materials - Mitchell	16
Thin Film Studies - Maggiore	22
Heavy Fermion Physics - Fisk	24
Mechanical Instability as a Solid-State Amorphization Mechanism - Koike	26
De Haas-van Alphen Effect and Fermi Surface of $\text{YBa}_2\text{Cu}_3\text{O}_{6.97}$ - Mueller	28
Bulk and Surface Electronic Structure of Transition, Rare-Earth and Actinide Materials - Boring	29
Lifetime of Localized Vibrational State in Solids - Clogston	31
Ultrasonic Studies - Leisure	33
Many-Body Calculations of Strongly Correlated Systems - Sham	34
Electron Structure of Films and Layers - Trickey	35
III. INTERDISCIPLINARY RESEARCH	36
Surface Modification of Materials - Nastasi	37
Laser Surface Processing - Jervis	41
Device Applications in Low-Dimensional Mixed-Valence Solids and Thin Films - Swanson	43
X-ray Absorption Spectroscopy Studies of High T_c Superconductors - Raistrick	45
Summary of Results on LAMPF Experiment 1235 Muon Level Crossing Resonance Spectroscopy - Cooke	48
IV. ADVANCED STUDIES PROGRAM	49

V.	NATIONAL HIGH MAGNETIC FIELD LABORATORY	53
VI.	SUMMER RESEARCH GROUP	55
VII.	VISITORS PROGRAM	57
VIII.	WORKSHOPS	59
IX.	CMS FACILITIES	62
	A. General Facilities	63
	CMS Office Facilities	
	CMS Office Transportables	
	B. Scientific Facilities	63
	Ion Beam Materials Laboratory	
	Electron Microscopy Laboratory	
	Mechanical Properties	
	Experimental Materials Science Facility	
	X-ray Machine Laboratory	
	Materials Science Laboratory	
X.	RESEARCH PUBLICATIONS AND PATENTS	67
APPENDIX A	CMS Seminars	97
APPENDIX B	CMS Visitors	104
APPENDIX C	CMS Sponsored Workshops	114
APPENDIX D	CMS Roster of Members, Affiliates Advisory Committees, Summer Research Groups, Consultants and Collaborators	193

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CENTER DIRECTOR'S OVERVIEW

Materials Community

The CMS mission is to enhance the contributions of materials science to the Laboratory's defense, energy, and scientific missions, and to build for a future of sustained excellence in materials science. The CMS is at the center of a growing and active intellectual communication in materials science that extends from basis research in condensed matter physics to applied materials research. Through its wide spectrum of programs, CMS is aggressively meeting this challenge. One simple way to describe the significance of the CMS impact on the Laboratory's materials science programs is to catalog the number of interactions between Laboratory staff, groups, and divisions and the CMS programs. A total of 196 divisional staff representing 31 groups and 12 divisions and centers participated in the CMS program. These organizations cover all five technical directorates and all of the technical organizations in the CM directorate. In addition to the 196 divisional staff, 30 CMS staff, including staff members, visitors, postdoctorals, and graduate students worked in the CMS for a grand total of 226 materials scientists participating in the CMS program. The body of this report describes the scientific content of the program.

Laboratory Fellow

Terry Mitchell was appointed to the rank of Laboratory Fellow this year. He was cited for his development and leadership of the Laboratory's electron microscopy community and his contributions to ceramics and high temperature superconductivity programs. Terry is an internationally recognized leader in materials science. He joins Fred Kocks and Zack Fisk as CMS Laboratory Fellows.

Distinguished Performance Awards

Three CMS staff received Distinguished Performance Awards for two separate activities this year. Carl Maggiore and Mark Hollander were part of a team including Joe Tesmer (P-10) and Caleb Evans (P-10) who was recognized for the development of the Ion Beam Materials Laboratory. Fred Mueller was part of a team recognized for developing explosive magnetic flux compression for doing de Haas van Alphen studies on high temperature superconductors.

CMS Facilities

Two major materials characterization facilities are central to the CMS program, the Electron Microscope Laboratory and the Ion Beam Materials Laboratory. Together these facilities serve a total of 129 user from the Laboratory and Universities. During this period, the potential impact of scanning tunneling and atomic force microscopy was recognized by the CM directorate and CMS was asked to develop with the participation of the CM technical organizations a central STM/AFM laboratory. A program, lead by Carl Maggiore, was developed for an STM/AFM facility and it will go into operation in FY92.

University of California Interactions

CMS developed several strong interactions with the UC this year. After working closely with the physics department at UCSD, a split position was offered to Zack Fisk where he remains a Laboratory employee for seven months of the year and takes a two thirds faculty position at UCSD for five months. With this arrangement, Zack will continue to lead his research program in Los Alamos and develop a program at UCSD. His expertise will contribute to both institutions and each will gain access to the capabilities and resources of the other.

The new UC Personnel Assignment Program (UCPAP) is an important mechanism to allow UC faculty and Laboratory staff to spend time at the respective institutions. During this CMS brought two Matthias Scholars to Los Alamos for UC, Lu Sham from UCSD and Rudy Wenk from UCB. This program worked effectively for all concerned.

Advanced Studies Program

The Advanced Studies Program finished with its second major workshop on high temperature superconductivity. This meeting was titled "Phenomenology and Application of High Temperature Superconductors" and was organized similar to the first workshop on theory of high temperature superconductors. The publication from this first workshop was so successful that it was a best seller in 1990 for Addison-Wesley.

The success of the ASP concept has lead to a decision to broaden the focus from superconductivity to the topic of correlated electron theory. The ASP program finished its job and a new program, containing many elements of the ASP will start next year. The Program in Correlated Electron Theory (PCET) will bring together the program fellows, many of the ASP fellows plus some new ones, Los Alamos staff, and UC faculty and students with a focus on correlated electron systems. This program promises to be as exciting scientifically as ASP plus it will be a major center of interaction between the Laboratory and UC.

National High Magnetic Field Laboratory

The NHMFL program, performed jointly with Florida State University and the University of Florida and funded by NSF, commenced its operation at Los Alamos this year. The main elements at Los Alamos are development of high field pulsed magnets and the development of high strength/high conductivity conductor to make high field magnets. Don Parkin, CMS Director, is one of the three principal investigators on the program and is leading the Los Alamos effort. The NHMFL as it develops over the next few years will be a significant element of the Laboratory's materials programs.

Materials Science Laboratory

The Materials Science Laboratory is a new 55,360 sq. ft. building that will provide state-of-the-art capabilities for the synthesis, processing, characterizing, and modeling of materials in support of the Laboratory's materials science programs. After many years of development and design, the ground breaking ceremony was held in July of this year. Construction is underway and the expected date for completion is for

the spring of 1993. The MSL will provide a scientifically interactive environment supported with modern facilities that will be the core of future developing materials research at Los Alamos.

I. INTRODUCTION

I. INTRODUCTION

This report summarizes the progress of the Center for Materials Science (CMS) from October 1, 1990 to September 30, 1991, and is the ninth such annual report. It has been a year of remarkable progress in building the programs of the Center. The extent of this progress is described in detail in the following pages of this report.

The CMS was established to enhance the contribution of materials science and technology to the Laboratory's defense, energy and scientific missions, and the Laboratory. In carrying out these responsibilities it has accepted four demanding missions:

- 1) Build a core group of highly rated, established materials scientists and solid state physicists.
- 2) Promote and support top quality, interdisciplinary materials research programs at Los Alamos.
- 3) Strengthen the interactions of materials science and Los Alamos with the external materials science community.
- 4) Establish and maintain modern materials research facilities in a readily accessible, central location.

The past year has been a very active one for CMS personnel.. We had three new visiting Matthias Scholars this year. Lu Sham, UC San Diego, was here from March thru August. He had a very fruitful stay working on the analysis of the ultrasound data generated by Al Migliori (P-10). Rudy Wenk, UC Berkeley, joined us in May, to work on characterization of geologic materials. He has been very active and interactive during his stay (ends in December). Finally, Ron Gibala, University of Michigan, joined us in September for an eight month visit.

Congratulations are in order for several CMS researchers. First, Terry Mitchell joins Fred Kocks and Zack Fisk in becoming a Laboratory Fellow. Next, Carl Maggiore and Mark Hollander, along with Joe Tesmer (P-10) and Caleb Evans (P-10), received a Distinguished Performance Award for their development of the Ion Beam Materials Laboratory into a world class materials characterization facility. Also, Fred Mueller was part of a six man team that received a Distinguished Performance Award for developing a high magnetic field compressive technique for doing de Haas van Alphen studies on complex materials.

We also have three new Postdoctoral Fellows bringing the total to eight this year. Alexander Balatsky from the Landau Institute in Moscow has joined CMS as a JRO Fellow to work on the theory of high Tc superconductors with theorists in T-11. Masahiko Inui from Stanford has also joined CMS to work on high Tc theory. They join Dermot Coffey in working in the Advanced Studies Program. Dermot will be leaving the program at the end of the year. Hisayuki Suematsu has joined us to work with Terry Mitchell and his team on materials characterization via electron microscopy. Jun Koike, who as a Postdoctoral Fellow in CMS the last two years developed a new method for amorphous phase formation, left this year for a permanent position at the University of Oregon. The other Postdocs who remained with us this year were Olle Eriksson (electronic structure),

Shuh-Rong Chen (constitutive relations), Li Luo (HTS films), and Sreeram Srinivasan (microstructure). We also have several new graduate students this year. Florian Heidelbach and Kristan Bennett are working with Rudy Wenk and the CMS staff this year. John Sarrao will be working with Zack Fisk and Al Migliori on resonance ultrasound problem.

Both of the CMS user facilities, the Electron Microscopy Laboratory and the Ion Beam Materials Laboratory, have very active schedule this year with many users. Also the X-ray Laboratory became fully operational this year with five machines. We have also began setting up a Scanning Tunneling Microscopy (STM) Laboratory which should be operational next year. Finally, there was a ground breaking ceremony for the new Materials Science Laboratory (55,360 ft²) and construction has begun.

II. CMS RESEARCH

POLYCRYSTAL PLASTICITY AND TEXTURE DEVELOPMENT

Principal Investigators: U. F. Kocks, CMS
S. R. Chen, CMS
A. D. Rollett, MST-6
M. G. Stout, MST-5
H. R. Wenk, CMS and UCB

Any anisotropy in the properties of normal, polycrystalline materials is primarily due to texture, i.e., preferred crystallographic orientations. A quantitative description requires two major steps: first, texture measurement and evaluation, and second, prediction of properties for any given texture. Beyond this capability at a given state of the material, one should be able to predict the future evolution of texture (and therefore of anisotropic properties) during plastic deformation. Finally, it is essential to verify such prediction by critical experiments. We have made major advances on all four of these fronts during the last year.

Texture Measurement and Analysis

First, methods for the analysis and representation of texture data have been established in collaboration with J. S. Kallend (Illinois Institute of Technology) and H.-R. Wenk (University of California/Berkeley) and have been collated into a coherent, rather wide-ranging set of software called "popLA: preferred orientation package - Los Alamos". Some of its capabilities are to correct experimental data sets, to analyze the symmetry properties of a given data set, to rotate, symmetrize, smooth and normalize them. Then, interpretations of the projections in terms of three-dimensional orientation space according to both the harmonic and WIMV methods can be obtained for samples of arbitrary symmetry, and of a crystal symmetry as low as orthorhombic. They are all accomplished (within a few minutes) on personal computers. Visual representation is achieved by various sections and projections of orientation space (in particular, in polar representations), using colors or grey-shades or contours. A most important capability is the transfer of orientation-space density information onto weights assigned to a number of discrete grains, which can then be used in computer simulations of anisotropic polycrystal properties. This technique enables the prediction of the future behavior of samples that are not initially isotropic, and a continual comparison of theory and experiment. The entire software package has been made available to the public, in the course of the Laboratory's efforts in Technology Transfer. It is being used at various universities and industrial laboratories.

Superconductors pose new challenges for texture analysis. Because of the low symmetry, diffraction peaks are weak and closely spaced. With a new approach it has been possible to determine a quantitative ODF of cold pressed 2223 powders with an extremely strong preferred orientation (Wenk and Phillips 1991). Also spurious peaks in pole figures from YBCO thin films could finally be attributed to diffraction on the substrate from continuous radiation. With truly monochromatic radiation they disappear (Wenk 1991). Heidelberg et al. (1991) have illustrated a quantitative relationship deposition temperature, texture and critical temperature of YBCO laser deposited films.

Prediction of Anisotropic Properties

The Los Alamos polycrystal plasticity (LApp) computer simulation code, which is also available in the popLA package in a PC version, has been augmented to treat crystals of lower symmetry and more general hardening laws. One of its uses is, based on an input of weighted grains files obtained from experimental texture data as evaluated by the WIMV method, to predict current anisotropic plastic properties. For this purpose, it is necessary to know the deformation modes available in the crystals, such as slip and twinning on various systems. For materials of lower than cubic symmetry, these are generally not known in any quantitative sense, such as the respective flow stresses as a function of temperature and composition. We have designed a method of deriving this information from a few macroscopic observations, such as the main rolling texture components. We have derived "deformation mode maps", which delineate domains of constant single-crystal yield surface topology under varying flow stresses for all the possible systems; within these domains, texture development tendencies remain constant. The method has been applied successfully to hexagonal materials such as titanium and zirconium and their respective alloys.

We have begun to initiate collaborative efforts with atomistic modelers to determine the Peierls stress in different slip systems: this could serve to predict relative slip systems activity.

The Effect of Texture Evolution on Strain Hardening

An extensive set of experiments on FCC and BCC metals and alloys has been initiated to verify general rules of plastic behavior, especially at high temperatures and high rates. The experiments have been completed for Cu polycrystals, at strain rates up to 1 s^{-1} and 700°C . In progress are experiments on stain less steel, and nickel; planned next is tantalum.

A significant aspect of these experimental verifications is their integration with texture measurements and calculated texture evolutions, which influence the strain-hardening rate, in some cases significantly. This complete treatment is (we believe) a first in mechanical properties testing.

Verification

Comparison with experimental experience has been a continuing feature of code development. Some key features have proven to be easy to match, others difficult. The most sensitive property, both from the point of view of measurement as from that of the assumptions used in predictions, is the polycrystal plastic potential: the strain-rate ratios at a given stress, for a whole spectrum of stress states. A broad set of new experiments on aluminum, copper, and nickel has been undertaken with this sensitivity in mind. One particular kind of these tests is the measurement of tension anisotropy in a rolled sheet ("Lankford coefficients", "R-values"). In some cases, continuing improvement of both testing and simulation procedure has now yielded satisfactory agreement; in others, there are still significant problems. It is imperative that these be ironed out before the simulations can be used routinely for engineering applications.

Materials with a very high rate sensitivity have been predicted to develop textures different from "normal" in some respects. Experiments have been undertaken to test this result on Al-2%Mg at high temperatures. An unexpected result has been that dynamic

recrystallization occurred in all cases where the rate sensitivity was high enough, and may in fact be primarily responsible for the observed differences in texture. This could, in itself, have interesting consequences.

Applications in Geophysics

H.-R. Wenk of the University of California at Berkeley is spending 8 months at CMS as a Matthias Scholar. This continues the collaboration that has been supported by IGPP for many years. He brought three of his graduate students to Los Alamos. Kirstin Bennett measured textures of experimentally deformed ice (by W. Durham at LLNL) by neutron diffraction at liquid nitrogen temperature (Bennett et al. 1991). Florian Heidelbach is developing a system to measure preferred orientation of individual grains with the scanning electron microscope and plans to apply it in a study of recrystallization in deformed rocks where local orientation differences are a crucial factor.

PLASTICITY LAWS AND PARAMETERS FOR ENGINEERING CODES

Principal Investigators: U. F. Kocks, CMS
 S. R. Chen, CMS
 W. J. Poole, McMaster University
 A. D. Rollett, MST-6
 P. J. Maudlin, N-6
 M. G. Stout, MST-5
 G. T. Gray III, MST-5
 P. S. Follansbee (MST-DO)

In Materials Science and Engineering, as in many other fields, some problems are so complex that "modeling" the various contributing processes in an integrated fashion is the most viable form of theoretical treatment. A model will typically incorporate both theoretical and empirical parts. Its aim is to describe and predict a chosen set of aspects of macroscopic behavior in the most reliable form possible. A number of practical constraints may interfere: one is that relevant material data are not available; another that, at least initially, very large amounts of computer time and memory may be necessary. We have made some attempts to overcome these problems, and are well on our way to establishing a viable model.

Two important aspects of materials behavior in plasticity that are not adequately accounted for in current engineering codes concern the kinetics and the anisotropy; the underlying mechanisms are known for both. For an effective description of the kinetics, the temperature and strain-rate dependence can be combined and expressed in terms of a few normalized variables, for both yield and strain hardening. The parameters for this model, and the extent of its applicability, are not well established for the high-temperature high-rate regime: they are being measured for a variety of cubic metals and alloys. Experimental results at medium strain rate should be applicable to higher rates at higher temperatures, within the same mechanism regime. An important aspect of these investigations is to establish boundaries in the "mechanism map" where additional processes occur or become dominant. Of particular interest in high-temperature deformation is the incidence of dynamic recrystallization, for which useful phenomenological descriptions are available.

Anisotropic behavior has been shown to be too complex and varied to be represented in the form of equations: numerical description are being established and implemented for cubic and hexagonal metals under multi-axial straining conditions. They are being applied (in collaboration with P. R. Dawson of Cornell University) to a quantitative treatment of three-dimensional deformation processing, including materials anisotropy, sliding and friction at external and internal boundaries, heat generation and flow, geometric and constitutive instabilities, changes in the microstructure (including by recrystallization, precipitation, resolutions, etc.), and prediction of product structure and properties, including surface finish and residual stresses.

Special problems arise in materials that are heterogeneous on a macroscopic scale, such as metal matrix composites. Here, the pattern of plastic flow can be non-uniform on a macroscopic scale - akin even to patterns of fluid flow through materials with embedded heterogeneities. This is a case where finite-element modeling on the microscopic scale has led to an increase in understanding that can, perhaps, eventually be condensed into new materials constitutive relations for heterogeneous materials. The non-uniform flow pattern leads also to significant materials rotations and different texture development.

Both the non-uniformity of flow and the texture development have been studied experimentally in Cu-W fiber composites tested in plane strain (in collaboration with J. D. Embury, McMaster University). It is planned to investigate the transformation between this "easy flow" and the more common problem of load transfer in composites, which occurs especially in uniaxial straining parallel to the fibers.

METASTABLE PHASES AND MICROSTRUCTURES

Principal Investigator: R. B. Schwarz, CMS

Introduction

Improvement in material properties often result from innovations in synthesis and processing methods. For example, microstructural refinements developed through processing can lead to improvements in both strength and ductility. These materials, however, are thermodynamically metastable and thus additional phases or defects are added to stabilize them against microstructural changes within the desired operational temperature range. Amorphous alloys are another example of materials with metastable phases and these have improved catalytic and magnetic properties.

A purpose of this research program is to provide fundamental knowledge on the interrelation between synthesis and processing and materials performance, with specific emphasis on materials with metastable structures. We investigate metallic and ceramic alloys (amorphous and microcrystalline) in thin film-, powder-, and bulk-form. Although the program is devoted to fundamental research, we maintain a close vision of the applied world by preferentially studying materials that are relevant to current-day engineering needs. We thus measure both the *microstructure* and the *properties* of metastable alloys.

Experimental Methods

We prepare alloys in thin film, powder, and bulk form. Thin films are formed by condensation in an ultra-high vacuum system. In these films we study the kinetics of solid-state transformations by in-situ electrical resistivity and Raleigh wave velocity measurements. After removing the films from the vacuum, we study their compositions and structure by x-ray diffraction, electron microscopy, and Rutherford back scattering.

We use mechanical alloying (MA), a high-energy ball milling technique, to prepare alloy powders with metastable structures. This technique enable us to prepare amorphous alloys and powders of intermetallics having grain sizes in the range of 515 nm. In our current study of tri-aluminides we start from mixtures of commercial elemental powders and we use hexane as a surfactant. The hexane prevents the agglomeration of the ductile aluminum powder and adds carbon in solid solution. During the consolidation of these powders by vacuum hot pressing, the carbon reacts with early transition metals in the alloys to form a fine and uniform dispersion of carbides. We can thus control both the morphology and volume fraction of precipitates during processing.

Synthesis of Novel Materials by Mechanical Alloying

Principal Investigators: R. B. Schwarz, CMS
S. Srinivasan, CMS
P. B. Desch, CMS
T. Mitchell, CMS
P. Nash, IIT, Chicago

MA is becoming an important technique for the synthesis of metastable powders (amorphous, noncrystalline, metastable phases, etc). We are using MA to synthesize powders of various intermetallics starting from mixtures of elemental powders. We consolidate these powders by hot pressing in vacuum or in argon. Finally, we characterize the microstructure and properties (mechanical, magnetic, catalytic, etc) of the compacts. Controlling all three processing steps, powder synthesis, powder consolidation, and characterization of the compacts (microscopic and macroscopic), enables us to feed-back on those aspects of the processing which are most important for the optimization of properties.

Ordered intermetallics generally possess attractive properties at high temperatures: high strength, low self-diffusion rates, and high elastic moduli. Ironically, the ordered structure also leads to brittleness in these alloys at near room temperature. The reasons for the brittleness varies with each system; low cleavage strength and grain boundary weakness are a couple of causes.

We are using MA to synthesize bulk polycrystalline intermetallics having one or more of these characteristics: (a) ultra-fine microstructures; (b) metastable crystalline phase(s); and (c) a fine and uniform dispersion of precipitates (carbides, oxides). Examples include (1) metastable $L1_2$ cubic phases of Al_3Ti , Al_3Zr , Al_3Hf , and ternary alloys based on these tri-aluminides; (2) Two-phase alloys of aluminum and Al_3Ti ; and (3) fine grained $MoSi_2$, $MoSi_2$ - WSi_2 alloys, and $MoSi_2$ - Mo_5Si_3 alloys.

Our preliminary mechanical test results are very encouraging. For example, a three-phase Al -18vol% Al_3Ti -8vol% TiC alloy, having grain sizes of about 200 nm and density of 2.96 g cm^{-3} , has a room temperature compressive strength of 610 MPa. At 500 °C, the strength drops to 100 MPa. The plastic strain to fracture exceeds 20% at all temperatures. These properties are comparable to those found in current advanced production Al - Cu alloys of higher density.

Our $MoSi_2$ -based alloys prepared by the MA synthesis route have smaller grain sizes and significantly lower oxygen content than those prepared by hot pressing commercial $MoSi_2$ powders. Minimizing the oxygen content in the powders is of utmost importance because (a) any SiO_2 at the surface of the powder particles is detrimental to the sintering process, and (b) following consolidation, the SiO_2 forms intergranular pockets which degrade the alloy's creep resistance. The lower oxygen content and the fine grains in our mechanically alloyed powders enabled us to reduce the customary pressing temperature by about 300°C, thus minimizing grain growth during consolidation while attaining an acceptable 97% relative density.

Future efforts will focus on relating the microstructure to the mechanical behavior of the alloys. The influence of the precipitates on mechanical properties and grain growth will also be thoroughly studied.

Kinetics of Solid State Reactions in Thin Films

Principal Investigators: R. B. Schwarz, CMS
J. B. Rubin, CMS

The study of glass formation in metallic thin films continues to be an active area for research. The interdiffusion reactions which underlay the formation and stability of amorphous alloys are of primary importance in determining what role these materials will play in any future commercial application. The thermodynamics of these solid-state reactions are reasonably well known, yet very little information exists concerning the kinetic factors. Such kinetic studies have been slowed by a lack of in situ analytical techniques, and the difficulty of making measurements during the first few minutes of these reactions.

We have developed an in situ electrical resistance method to examine crystal $\pm$ amorphous transformations in thin films. This technique incorporates a temperature-measurement and control system combining ultra-rapid response with an extremely high level of stability. The method is being applied to initially crystalline, multilayered Ni/Zr films to elucidate the amorphization mechanism for very short reaction times and to derive diffusion data in amorphous alloys. Coevaporated, initially amorphous films are also being studied to define the regions of metastable phase equilibria and the Glass Forming Range (GFR). The GFR data is used to evaluate and refine existing kinetic models of glass formation (in collaboration with).

A second in situ technique is under development to measure the elastic properties of sub-micron metallic films. This method uses phase-detection of acoustic surface waves (Raleigh waves) to probe the shear modulus of the films. The experimental arrangement is sensitive to $< 0.01\%$ modulus change. The temperature measurement and control system described above is also included so that changes in mechanical behavior can be examined during crystalline $\leftrightarrow$ amorphous transformations in Ni/Zr alloys. The differences between the elastic moduli of thin films synthesized by solid-state interdiffusion reactions and by coevaporation, in conjunction with x-ray diffraction and TEM data, will provides us with information on the relative atomic-scale structure of the films produced by these two preparation techniques.

These two in situ methods, although currently applied to amorphization reactions, can be used in the study other materials problems such as the supermodulus effect, order-disorder transformations, precipitation reactions, and phase changes in superconducting films.

Metastable Phase Formation in Al-Ge Alloys by Mechanical Alloying

Principal Investigators: R. B. Schwarz, CMS
P. J. Yvon, CMS
D. Schiferl, M-6
W. L. Johnson, Caltech

Aluminum and germanium form a simple eutheic system ($T_e = 421^\circ\text{C}$, $x_e = 0.3$) with little mutual solubilities. Because elemental aluminum and germanium have metallic and covalent bonding, respectively, it is not surprising that investigators have reported the formation of metastable Al-Ge phases by the rapid solidification of melts. We are investigating the formation of metastable phases in Al_{1-x}Ge alloy powders prepared by mechanical alloying (MA). We are also investigating phase transitions in these powders induced by high hydrostatic pressures (> 10 GPa).

The synthesis of $\text{Al}_{1-x}\text{Ge}_x$ by MA yielded some puzzling results: for $0.4 < x < 0.75$, differential scanning calorimetry reveals two endothermic peaks. The first occurs at 421°C and corresponds to the expected eutheic reaction of aluminum and germanium. This peak decreases in intensity and disappears for $x = 0.75$, instead of $x = 0.99$. The second peak, at 515°C , appears at $x = 0.4$ and increases in intensity reaching a maximum for $x = 0.75$. X-ray diffraction of as mechanically-alloyed powder shows similarly puzzling results: with increasing x , the Bragg peaks of aluminum decrease in intensity and disappear completely at $x = 0.75$. The disappearance of the eutheic reaction may be attributed to: (a) an increase in the solubility of aluminum in germanium as a result of MA, and/or (b) the formation of a thin aluminum layer (possibly monoatomic) surrounding each germanium grain. The second transformation (515°C) cannot be explained by the equilibrium phase diagram nor corresponds to any of the metastable phases produced by rapid solidification, reported previously. This reaction is reversible and thus cannot be studied by room-temperature x-ray diffraction. We will be using a TEM hot stage to further investigate this reversible phase transition, apparent only in Al-Ge alloys prepared by MA. Concurrently to these studies, we are investigating crystal-to-amorphous phase transitions induced by high pressures on alloy powders prepared by MA.

INTERFACES AND OTHER DEFECT IN MATERIALS

Principal Investigator: T. E. Mitchell, CMS

Introduction

Internal interfaces play a critical role in the physical and mechanical properties of ceramics. Such interfaces include both intergranular and interphase boundaries, which can also be termed homophase and heterophase boundaries. The first case encompasses grain and twin boundaries where there is only an orientation change. In the second case both the structure and orientation can change across the interface. There may be a special orientation relationship, as in epitaxially grown structures, or no orientation relationship at all, as in ceramic-ceramic composites. In both types of boundaries, segregation of impurities and boundary phases are common. Transmission electron microscopy, both high resolution and analytical, is one of the most powerful techniques for characterizing interfaces. The CMS electron microscopy facility provides such an opportunity.

Experimental Methods

Interfaces in a variety of ceramic materials have been studied by transmission electron microscopy (TEM), as described below. For layered and coated materials both plane sections and cross-sections have been employed. Techniques for preparation of cross-sectional TEM specimens are tricky and have to be tailored to the particular system. For example, epitaxially-grown layered systems tend to have good adhesion and can be prepared by standard sandwich methods. On the other hand, coated systems such as zirconia thermal barrier coatings often have poor adhesion at the interface and need special handling for mechanical thinning and ion milling. Ion milling was performed on a Gatan ion mill equipped with a liquid nitrogen specimen cooler which is important for minimizing the damaged region in specimens for high resolution electron microscopy (HREM). HREM was performed on a Philips CM30ST with a point-to-point resolution of 1.9Å while analytical microscopy (AEM) was done on a separate CM30 equipped with a Kevex x-ray system and a Gatan parallel EELS system.

OXIDE SUPERCONDUCTORS OF ELECTRON MICROSCOPY

Principal Investigators: T. E. Mitchell, CMS
 R. Gronsky, LBL
 G. Van Tendeloo, Universitat Antwerpen

Defects are known to play a critical role in the current carrying capacity of conventional superconductors and are equally important in high T_c oxide superconductors. The only way that the nature and spatial distribution of such defects can be determined is by transmission electron microscopy (TEM). The advantage of TEM is that it is possible to combine various imaging modes with electron diffraction and other analytical techniques such as x-ray energy dispersive spectrometry (EDS) in order to characterize defects structurally and chemically. Important defects in oxide superconductors include point defects, impurities, dislocations, stacking faults, twins, grain boundaries and second Phases. In this article we will describe the various techniques and their application to the study of defects in the oxide superconductors. As each new oxide superconductor has been discovered over the past few years, it has been subjected to intense structural and microstructural analysis of TEM. A wealth of information about crystal chemistry, phase transformations and defect structures has emerged from such studies, both as fundamental studies in their own right and as attempts to correlate with the superconducting transition temperature (T_c) and the critical current density (J_c).

MICROSTRUCTURE OF EPITAXIAL $\text{YBa}_2\text{Cu}_3\text{O}_7$ THIN FILMS

Principal investigators: T. E. Mitchell, CMS
 S. N. Basu, Boston University
 A. Carim, Penn State University
 M. Nastasi, MST-7
 R. Muenchausen, ERDC
 I. Raistrick, MEE-11

Thin epitaxial films of $\text{YBa}_2\text{Cu}_3\text{O}_7$ on single crystal substrates have been prepared in situ by laser ablation and by post situ annealing of evaporated films of Cu, Y and BaF_2 . Substrates include (001) SrTiO_3 , LaGaO_3 , and LaAlO_3 . For both in situ and post insitu annealed films, epitaxial (001) grains of $\text{YBa}_2\text{Cu}_3\text{O}_7$ from near the substrate but (100) and (010) grains tend to nucleate for thicknesses greater than $\sim 0.5 \mu\text{m}$. 90° grain boundaries are therefore common, as well as other defects such as small angle boundaries, dislocations and stacking faults. high resolution electron microscopy of the substrate/superconductor interface shows regions of perfect epitaxy, distorted areas, amorphous regions and areas of interdiffusion. The relationship of observed microstructure to critical current density is discussed.

STRUCTURAL CHANGES OF $\text{Bi}_{1.8}\text{Sr}_2(\text{Ca}_{1-x}\text{Y}_x)\text{Cu}_{2.2}\text{O}_z$ CERAMICS WITH YTTRIUM CONTENT STUDIED BY ELECTRON DIFFRACTION AND HIGH-RESOLUTION ELECTRON MICROSCOPY

Principal Investigators: Takashi Onozuka, Tohoku University
Hiroshi Sato, Purdue University
T. E. Mitchell, CMS

The mode of the incommensurate modulation in the b direction of the $\text{Bi}_{1.8}\text{Sr}_2(\text{Ca}_{1-x}\text{Y}_x)\text{Cu}_{2.2}\text{O}_z$ ($0.05 < x < 0.75$) system is investigated by means of electron diffraction and high-resolution lattice imaging. The change of period of the long-period structure with x is found to be basically due to the mixing ratio of domains of two modulations periods with $b = 4.5b_0$ and $5b_0$ or $4.5b_0$ and $4b_0$, $a \approx b \approx b_0$ (0.54 nm) and $c \approx c_0$ (3.1 nm). The change of the mixing mode from one to the other mentioned above occurs just in the yttrium concentration range, $0.45 < x < 0.65$, which also corresponds to the superconductor (metallic)-to-semiconductor transition boundary. The mixing modes of the domains are directly recorded as a contrast modulation with half periods, $4.5b_0/2$ and $5b_0/2$ or $4.5b_0/2$ and $4b_0/2$ in high-resolution lattice images. These images are reproduced well by a multislice computer-simulation technique.

DISLOCATION ARRANGEMENTS IN $\text{GaAs}/\text{Ga}_{1-x}\text{In}_x\text{As}$ MULTILAYERS GROWN ON (001), (111) AND (112) SUBSTRATES

Principal Investigators: T. E. Mitchell, CMS
O. Unal, CMS and CWRU

$\text{GaAs}/\text{Ga}_{1-x}\text{In}_x\text{As}$ strained layer superlattices with well-widths of 7nm, barrier widths of 14 nm and periods of 10 to 30 have been examined by transmission electron microscopy in plan view and in cross-section for (001), (111) and (211) substrates. Individual layers are below the critical thickness while the overall SLS's are above the critical thickness for dislocation generation. (001) substrates give rise to square grids of 60° dislocations lying parallel to $\langle 110 \rangle$ with inclined $1/2\langle 101 \rangle$ Burgers vectors, resulting from dislocations motion on 8 slip systems. (111) substrates give triangular networks 60° dislocations lying parallel to $\langle 110 \rangle$ resulting from motion on 6 slip systems. (112) substrates have two sets of primary dislocations lying along $\langle 132 \rangle$ directions, along with secondary 60° dislocations lying along $[110]$. Long Lomer-Cottrell with Burgers vectors lying parallel to the substrate/SLS interface are occasionally observed for (001) substrates, while short segments are observed for (112) substrates; these are formed by reaction between conjugate dislocations. These dislocations arrangements are discussed in terms of the resolved shear stresses resulting from epitaxy for the various substrates orientations. Dislocation densities are much less than those required for complete strain relief. This is analyzed in terms of the reduction in the stress acting on dislocations from partial strain relief, along with a friction stress due to a combination of the Peierls stress and solution hardening from the In substitution. A friction stress $\sim 10^{-3}\mu$ is required to explain the observed densities (μ is the shear modulus).

CVD Si_3N_4 ON SINGLE CRYSTAL SiC : II, HIGH RESOLUTION ELECTRON MICROSCOPY AND ATOMIC MODELS OF THE INTERFACE

Principal Investigators: O. Unal, CMS and CWRU
T.E. Mitchell, CMS

Interface studies of CVD Si_3N_4 on (111) SiC single crystal substrates have been made by transmission electron microscopy (TEM). It is found that there are two orientation relationships both of which involve the same (1010) Si_3N_4 /(111) SiC planar relationship. However, the orientation relationships are not perfect and rotations of 2-6° are commonly seen between both directions and planes involved. High resolution electron microscopy (HREM) of the interfaces show that the SiC and Si_3N_4 are continuous up to the interface and that no intermediate phases are formed. However, due to the small rotations, the HREM images are difficult to interpret directly in terms of atomic positions. Nevertheless, possible atomic models of the interface are proposed based upon the experimental findings. These models exploit the similarities between SiN_4 and SiC_4 tetrahedra in Si_3N_4 and SiC , respectively. The observed orientation relationships appear to be due to matching of tetrahedra across the interface along with adequate lattice matches.

{112} <111> TWINS IN TETRAGONAL MoSi_2

Principle Investigators: T. E. Mitchell, CMS
R. G. Castro, MST-6
M. M. Chadwick, MST-6

Plasma-sprayed tetragonal MoSi_2 has been examined by transmission electron microscopy. Growth twins are commonly observed in the microstructure. Analysis of diffraction patterns using a stereographic projection indicates that the twinning plane is {112} and the twinning direction is <111>. Atomic modelling of the twin interface shows that a key element is the pseudo-hexagonal nature of the {110} MoSi_2 planes which allows a $\Sigma 2$ coincidence site relationship between matrix and twin. The habit plane for the twins is commonly observed to be {110}, implying that the plane corresponds to a twist boundary. The rotation angle is almost exactly 60°. It is likely that the twins result from the hexagonal-to-tetragonal transformation of MoSi_2 at high temperatures.

THE MICROSTRUCTURE OF TITANIUM BERYLLIDE, TiBe_{12}

Principle Investigators: D. Banerjee, Defense Metallurgical Research Lab.
L. Jacobson, Ford Motor Co.
J. Zindell, Ford Motor Co.
T. E. Mitchell, CMS

titanium beryllide (TiBe_{12}) has been processed by various techniques, including inert gas arc melting, sputter deposition and as second phase particles in atomized powder of alloys ranging in composition from 1 to 35 weight percent Ti. The TiBe_{12} that formed in the various alloys was characterized by transmission electron microscopy. Defect structures such as microtwinning, antiphase domain boundaries and dislocations have been observed within the beryllide phase. Descriptions of these defect structures will be presented in this paper, together with a discussion of their origin.

Introduction

A recent renewal of interest in the intermetallic compounds of beryllium with transition metals has become evident. Earlier work demonstrated the low densities, high melting temperatures, good high temperature mechanical properties and excellent oxidation resistance of these compounds. This paper treats the intermetallic TiBe_{12} , as made by several methods, including inert gas arc melting, sputtering and atomization of dilute alloys of beryllium and titanium. The TiBe_{12} compound has a complex body centered tetragonal unit cell (14/mmm), with 26 atoms, and is isostructural with other compounds such as MoBe_{12} and NbBe_{12} . Our interest in the titanium compound arose mainly from the use of titanium as an alloying additive to beryllium, in which it forms a stable dispersion of intermetallic particles upon rapid solidification.

Experimental

Cast beryllide samples were prepared by arc melting in an argon atmosphere, with a minimum of three melts to improve homogeneity, and slow directional cooling on the last melt in order to minimize porosity and generate as much volume of single phase compound possible. The target composition for the cast sample examined in this study was Be-20wt%Ti, a composition intended to avoid forming the compound $\text{Ti}_2\text{Be}^{17}$. Rapidly solidified alloy powder with aim composition of Be-2wt%Ti was prepared by centrifugal atomization into a helium atmosphere. The powder was consolidated by hot isostatic pressing. Sputter deposited films, supplied by Aerospace Division of Martin Marietta, were made by co-depositing Be and Ti on a substrate maintained at a temperature of at least 500°C. Aim composition of the foil used in this study was Be-35wt%Ti.

HIGH DOSE NEUTRON IRRADIATION DAMAGE IN ALPHA ALUMINA

Principal Investigators: R. A. Youngman, BP Research
T. E. Mitchell, CMS
F. W. Clinard, Jr., MST-4
G. F. Hurley, MST-4

Bulk samples of single crystalline and polycrystalline alpha alumina have been neutron-irradiation in the Experimental Breeder Reactor-II (EBR-II) to doses of 10^{26}n/m^2 at temperatures of 925K and 1100K. The samples were found to swell macroscopically between 3% and 6% depending on the temperature of irradiation and the form of the materials. The damage microstructures were investigated via transmission electron microscopy in order to understand the origin of the macroscopic swelling. In both single crystals and polycrystals the damage consists of a high density dislocation structure containing predominantly $b = 1/3 \langle 1011 \rangle$ dislocation loops on the (0001) planes coexistent with a high density of voids which are aligned along the c-axis in this rhombohedral material. The established theory of void formation in metals is utilized to explain the formation of voids in alumina. The polycrystalline samples were extensively micro-cracked and this is thought to be due to anisotropic swelling of the grains which in turn leads to stresses and fracturing at the grain boundaries.

Thin Film Studies

Principal Investigators:

L. Luo, CMS
 R. Muenchausen, ERDC
 J. Jimenez, Rensselaer Polytechnique
 L. Schowalter, Rensselaer Polytechnique
 A. Kaloyeros, SUNY Albany
 M. Nastasi, MST-7
 T. Inoue, Iwaki Meisei University
 C. Maggiore, CMS

The original justification for this work was to develop fabrication techniques for producing hybrid superconductor-semiconductor devices. There is a fundamental incompatibility between the high temperatures required to grow good quality high temperature superconducting material and the diffusion of Si from the substrate into the superconducting film. The use of buffer layers to prevent interdiffusion depends on proper chemistry to minimize reactions at the interface and matching crystallography to allow epitaxial growth. We have expanded the effort to include a wider variety of films, substrates, deposition techniques, and buffer layers.

A new insulating buffer layer, CeO_2 , has been identified for use between YBCO and Si. Cerium dioxide is an interesting buffer material because of its chemical stability and close lattice match with silicon. The CeO_2 which is deposited by electron beam evaporation in an oxygen environment grows on Si(100) in the (110) orientation. There is a non-uniform amorphous layer at the silicon interface similar to that observed when YSZ is grown on Si. The CeO_2 buffer layer has proven to be a suitable substrate for deposition of *a*-axis oriented YBCO. A superconducting transition temperature of 87 K and critical current density of $1.5 \times 10^5 \text{ A/cm}^2$ at 75 K have been measured. This is the highest reported value for *a*-axis oriented YBCO films.

Another alternative deposition technique that may be appropriate for direct growth without a buffer layer is based on chemical vapor deposition. By controlling the substrate temperature during deposition, thermally induced substrate damage and substrate/film chemical interactions may be reduced. The technique appears to show some promise for the growth of YBCO on substrates of MgO, silver, and sapphire. An initial high substrate temperature leads to the formation of a highly *c*-axis oriented "seed" layer which provides a template for lower temperature growth that minimizes substrate interactions.

In general, CVD is a very attractive approach because it can be adapted to large area and non-planar surfaces. Unfortunately the resulting films are often inferior to the physical vapor deposition techniques such as laser ablation, sputtering, or molecular beam epitaxy. Microwave radiation can be added to ordinary metalorganic vapor deposition to enhance the process by creating a plasma. This has been used to grow (100) BaTiO_3 on (100) LaAlO_3 and (100) NdGaO_3 . The interface is atomically abrupt with periodic dislocation arrays due to the large lattice mismatch.

We have also developed a method for producing oriented single crystal metallic disilicide on an amorphous layer of SiO_2 on a single crystal silicon substrate. The process takes advantage of the SIMOX (Silicon-on-insulator formed by IMplantation of Oxygen)

process to produce a thin single crystal Si layer on top of a buried layer of amorphous silicon dioxide. An overlayer of Ni is evaporated on the wafer of sufficient thickness to completely react with the Si layer. Subsequent annealing converts the layer to single crystal NiSi_2 and the disilicide is oriented relative to the substrate.

HEAVY FERMION PHYSICS

Principal Investigator: Zachary Fisk, CMS

Hybridization Gap Materials

We have completed an extensive set of measurements on the small gap material $\text{Ce}_3\text{Bi}_4\text{Pt}_3$, a cubic compound we discovered via flux growth experiments. These measurements include specific heat, electrical resistivity, Hall effect, magnetoresistivity, lattice parameter versus temperature and neutron inelastic scattering to observe the gap. The influence of chemical substitution on various of these properties was also examined. This compound is one of only three such compounds of Ce known, in which a Kondo-type interaction leads to semiconducting behavior, the neighboring rare earth compound analogues being metallic. We have a qualitative theory for our observations based on Kondo ideas. There is much interest in such compounds in the condensed matter community both from the standpoint of metal insulator transitions and topological changes in Fermi surface characteristics due to electron correlation effects.

High- γ Materials

A continuing study involves YbBiPt , a cubic, half-Heusler intermetallic which appears to have the largest known γ for any intermetallic compound, 8J/mole-Yb K^2 . We have found an unusual phase transition in this compound at $.4\text{K}$, with some of the characteristics of a spin glass, something not to be expected in a chemically ordered material. In order to achieve such a large γ , other competing interactions must be on the same scale as the Kondo scale, which is of order 1K here. We have argued why this appears to be the case in our compound, and this suggests fruitful avenues for the search for other such intermetallics. One of the interesting aspects of YbBiPt is that the background carrier count appears to be that of a semi-metal, indicating that the mass enhancement is exceptionally large in this case.

High T_c Superconductivity

Principal Investigator: Zachary Fisk, CMS

Neutron Scattering Collaboration

Collaborative experiments with G. Aeppli of Bell Laboratories have been completed on Sr-doped La_2CuO_4 . These have investigated the magnetic response of the metallic state, and show the presence of spin-wave features about certain Bragg points in reciprocal space. This work has been in progress for several years and has now been published in Physical Review Letters this September.

EPR in Cuprates

A collaboration with S. Oseroff (San Diego State) on Gd-doped La_2CuO_4 EPR has been completed and is being written up. The spectra are amazingly complicated but are now completely understood. The crystal field Hamiltonian necessary to fit the data involves a large strain term coming from the magnetically ordered CuO_2 -planes, and has not been

directly observed by any other measurements. The importance of the work is that it gives a microscopic characterization of the La-site in this cuprate, an important ingredient for understanding these complicated materials.

Resonant Ultrasound on Sr-doped La_2CuO_4

The resonant ultrasound collaboration with A.Migliori on the La_2CuO_4 -based single crystals has continued to Sr-dopings of 0.2. These experiments have tracked the elastic constant softening at the orthorhombic-tetragonal with doping, and a ferro-electric type soft-mode model has been used to fit the data. This work has also resulted in a Physical Review Letter this year. The interesting possibility raised by the experimental results and their interpretation is that important non-linear electron-phonon interaction may be crucial to high T_c .

MECHANICAL INSTABILITY AS A SOLID-STATE AMORPHIZATION MECHANISM

Principal Investigator: J. Koike, CMS

Some intermetallic compounds and semiconductors undergo a crystalline to amorphous phase transformation during irradiation with energetic particles. Before amorphization takes place, a large volume increase and associated shear modulus softening have been reported. Based on these observations and similarities to what have been observed upon melting, the mechanical instability of a crystalline lattice has been suggested to be a mechanism for irradiation-induced amorphization. Similar volume increase was observed before amorphization by ion implantation, hydrogen charging, and mechanical deformation, and associated softening of the elastic moduli is expected.

In this theoretical work, static displacement of lattice atoms was considered as a manifestation of any type of lattice defects ultimately leading to amorphization. The squared displacement amplitude was assumed to be proportional to the concentration of lattice defects. Calculation of fractional increase of the interatomic distance (Q) showed that there are critical values for Q and the defect concentration above which a crystalline state is considered to be unstable. In most cases, the critical value of Q is found to be approximately 0.5% depending on the mass, density, initial elastic moduli of the material, and the driving force for amorphization. At the critical Q value, decrease in elastic moduli is found to be 65%, independent of the material. These values are in good agreement with experiment.

The results indicate a striking similarity to melting as described by Lindeman's criteria in that the crystalline structure becomes unstable when the interatomic distance increases to a critical value. In the case of amorphization, this can be achieved by static displacement of lattice atoms introduced in the crystal by means of, for example, ion irradiation, ion implantation, hydrogen charging, and mechanical deformation. In conjunction with a significant decrease in the elastic moduli, amorphization can be viewed as catastrophic collapse of the crystalline structure caused by the mechanical instability.

A UNIQUE ELASTIC BEHAVIOR OF PARTIALLY AMORPHIZED NiTi PRODUCED BY COLD ROLLING

Principal Investigators: J. Koike, CMS
H. W. Sizek, MST-5

We have previously reported that an amorphous phase can form during cold rolling of NiTi intermetallic compound. Investigation of microstructure with transmission electron microscopy indicated that the driving force and the transformation mechanism are, respectively, the elastic energy and the mechanical instability, originated from dislocation accumulation.

Our current activity has been focused on a mechanical property associated with the peculiar microstructure of cold-rolled NiTi, which is composed of a very strong but brittle amorphous phase in an easily deformable crystalline matrix. Tensile test of this "composite" material showed the same stress-strain curve for both loading and unloading up to a fracture point (a stress of 1.9 GPa and a strain of 14%). This "hyperelastic"

behavior has been further studied by examining the annealing effects on the microstructure and the mechanical property. Annealing at 275°C (above the austenite transformation temperature) did not alter the "hyperelastic" behavior. While, annealing at 550°C (above the crystallization temperature of amorphous NiTi) altered the mechanical property to the original one observed before cold rolling. These results indicate that the "hyperleastic" behavior is caused by inclusion of an amorphous phase. Detail explanation of the phenomenon will be sought by performing quantitative experiments.

ELECTRON IRRADIATION EFFECTS OF DIAMOND

Principal Investigators: J. Koike, CMS
T. E. Mitchell, CMS
D. M. Parkin, CMS

Recent progress in synthesizing diamond thin films has opened a possibility of utilizing diamond as a component of semiconductor devices. Ion beam technology is expected to be extensively employed in conjunction with diamond thin films as has been the case for conventional semiconductors. However, irradiation damage in diamond is not well understood. The purpose of this work is to provide basic information regarding irradiation response of diamond.

Type Ha natural diamond was irradiated with high energy electrons in Philips CM30 electron microscope. Observation of defect cluster formation at different electron energy indicated that the displacement threshold energy is 37.5, 45.6, and 47.6 eV in the $\langle 100 \rangle$, $\langle 110 \rangle$, and $\langle 111 \rangle$ directions, respectively. Irradiation at different temperature revealed that defect clusters can form even 16 K. Interstitials were found to be mobile above 50 K. Further work is underway to determine the activation energy for point defect migration.

DE HAAS-VAN ALPHEN EFFECT AND FERMI SURFACE OF YBa₂Cu₃O_{6.97}

Principal Investigators:

F. M. Mueller, CMS
C. M. Fowler, M-6
B. L. Freeman, M-6
W. L. Hults, ERDC
J. C. King, M-6
J. L. Smith, ERDC

The high temperature ceramic superconductors (HTSC) have generated substantial scientific and technical interest. Perhaps the chief basic questions of interest to researchers are what is the superconductivity mechanism what is the nature of these materials in their normal phase at low temperatures? A direct ground state measurement such as the de Haas-van Alphen (dHvA) effect gives a direct answer to the latter question: If the susceptibility shows oscillations, periodic in $1/B$, the magnetic induction, then the material exhibits a fermi surface. Measurements of the dHvA effect using 100 T fields and temperatures below 4.2K. The basic data obtained is the oscillatory part of the YBCO magnetization as a function of applied field. As least three well-defined frequencies have been deduced from these data. We have reported preliminary results and recently there has been a report of dHvA oscillations for YBCO by Kido et al. using fields up to 27 T. As is discussed below, their oscillatory frequency of 0.54kT is virtually identical with our lowest observed frequency.

Our experiments are carried out in large pulsed fields, and this puts a number of rather severe constraints on the preparation of the samples as well as the measurement techniques. The samples are in the form of fine-grained powders embedded in a non-conducting medium so that pulsed magnetic fields can easily penetrate between and into the grains during the time of the pulse. The YBCO samples exhibited a T_c onset of 93 K. The techniques used to prepare and characterize the YBCO samples has been discussed. Superconducting powder was well stirred into epoxy and allowed to harden for 12 hours in a 4.2T field, oriented along the cylindrical axis. This technique produced samples which maintained a c-axis orientation along the magnetic field axis to better than two degrees as seen by x-rays and NMR. The sample density (17% by volume) is well below the percolation retardation by eddy current effects in some detail. The thermal rise due to these effects in a typical dHvA experiment is estimated to be no bigger than 0.2K for our YBCO powder.

This work has been presented at a number of meetings over the last 2 years in poster, contributed and invited sessions. It was the basis for a LANL small-team distinguished performance award. The focus on this team is shifting to measurements of the type II superconducting transition field, B_{c2}. Several preliminary experiments have been already carried out, suggesting that B_{c2} along the c axis (these materials are highly anisotropic, and the c axis critical field is believed to be the smallest) is higher than 100 tesla or 1 mega gauss. Modifications of the field generators to bring them above 100 tesla has already been successfully tested.

BULK AND SURFACE ELECTRONIC STRUCTURE OF TRANSITION, RARE-EARTH AND ACTINIDE MATERIALS

Principal Investigators:

O. Eriksson, CMS
A. M. Boring, CMS
J. M. Wills, T-1
R. C. Albers, T-11
L. E. Cox, NMT-5

The electronic structure and related properties, of both bulk as well as surfaces, are being investigated by means of first principles calculations. The main emphasis is on transition metal, rare-earth (Ce), and actinide systems. This effort is performed in conjunction with a host of experimental programs at the Laboratory. One main motivation is to compare and understand both transition metal systems, as well as the more complicated f-electron materials, and to determine what determines the similarities in some ground state properties, *e.g.*, the equilibrium volumes, and the differences in others, *e.g.*, the crystal structures. We are also trying to predict novel materials behavior, with new and interesting properties, *e.g.*, magnetic overlayers.

The computer codes used in these studies can handle both surface as well as bulk geometries. The work was also done using various levels of approximation:

- i) spherically averaged potentials (LMTO-ASA)
- ii) spherically averaged potentials inside muffin-tin spheres but full warping in the interstitial (the surface code)
- iii) no shape approximation to the charge density or potential (the bulk full potential code)

This gives the flexibility to do both highly accurate calculations (bulk full potential), as well as very fast, but less accurate, calculations (LMTO-ASA). Some of these codes have (partly) been developed at the Laboratory. For instance a large part of the bulk full potential code written at the Laboratory, in order to optimize speed and accuracy, for use in some of our efforts on crystal structure stabilities on rare-earths and actinides (see below). Also, the spin-orbit interaction was incorporated in the surface code, while maintaining the possibility to perform spin polarized calculations. Therefore both spin and orbital moments can now be calculated for surface geometries. Furthermore, the tsurface code was modified to be able to calculate the total energy as a function of a Lagrangian parameter, the magnetic moment. These so called fixed spin moment calculations were used to predict new magnetic properties of surfaces. We believe it important to have a non-constrained description of the charge (and spin) density as well as potential at surfaces and we are currently modifying the bulk full potential code to handle surface geometries.

Elements

We have during the last year studied the crystal structure stabilities of Ce and the early actinides (Th, Pa and U). We have also studied the crystal structure of delocalized Am. We have shown that for all these systems the onset of low symmetry crystal structures is driven by the contribution of the f electrons. This gives rise to a quite complicated ($T = 0$) phase diagram in Ce, which our calculations reproduce (PRL 67, 2215, 1991). Our calculations also reproduce the experimentally observed crystal structures in the early actinides as well as in the high pressure phase of Am. A continuation of this investigation is our present study of the crystal structure stabilities of Np.

We have also extended our previous calculations of orbital magnetism in the 3d elements (Fe, Co, and Ni) to alloys formed between these systems. The calculations show that, in agreement with experimental data, the orbital contribution represents between 5-15% of the total moment.

Surfaces

Using a model system of an ideal Ag substrate with a monolayer of Rh on top, we have pointed out the possibility of ferromagnetism in the chemisorbed top layer (PRL 66, 1350, 1991). This represents a novel material, since 4d magnetism is very uncommon (only a couple of other examples exist). Recent experimental work has been supportive to this prediction. We have also calculated the spin and orbital moments of Mn, Fe, Co, and Ni, and shown that whereas the surface enhancement of the spin moment can be as big as ~35%, the enhancement of the orbital moment is sometimes more than 100%. Furthermore, we have, together with recent XPS measurements at the Laboratory, predicted that the surface of α -Pu is more like an other allotrope, namely the δ -phase. This is similar to the prediction we did last year, that the electronic structure of the surface of α -Ce is like the electronic structure in γ -Ce, something which was later verified experimentally. Also, surface electronic structure calculations of bcc uranium, have reproduced the experimentally observed workfunction.

Compounds

Some recent experiments, partly done at the Laboratory, showed that NiI_2 is a typical Mott insulator. We have, in collaboration with Per Soderlind at Uppsala University, performed calculations on this system, and have reproduced an insulating (semiconducting) ground state as well as the magnetic moment.

Other experimental efforts have shown that the transport properties of the RBiPt ($\text{R} = \text{Y, Nd} - \text{Lu}$) compounds change drastically as the series is traversed. These systems are semiconducting for R being an early rare-earth element, but metallic for YbBiPt and LuBiPt . We have performed calculations of these systems, and our calculations reproduce the experimental findings. The closing of the semiconducting gap in YbBiPt and LuBiPt is found to be governed by the smaller volume for these compounds.

LIFETIME OF LOCALIZED VIBRATIONAL STATES IN SOLIDS

Principal Investigators: A. M. Clogston, CMS
H. Kieth McDowell, CLS-2

Molecular crystals composed of two (or more) nonlinearly coupled vibrational systems introduce an important new class of many body problems into the physics and chemistry of the solid state. Much of the recent work in the area has focused on long, pseudo one-dimensional chains of molecules which support a system of acoustic vibrations/phonons (i.e. sound waves) nonlinearly coupled to high frequency (i.e. infrared) optical vibrations/phonons. The interest in such systems derives from their potential for forming long-lived localized vibrational states. These are states where the acoustic and optical vibrations interact in such a way as to produce a localized region of vibrations which may or may not move through the crystal. If the lifetimes of such states are sufficiently long, they can play a significant role in the thermodynamics of the crystals and may represent an important mechanism of energy transport. Theoretical and experimental interest has therefore focused on the lifetime of these localized vibrational states. Important areas of application could be to biological molecules and explosives.

Coupled vibrational states of the sort described above are usually occupied by only a few quanta of energy and therefore must be treated quantum mechanically. Furthermore, since the lifetimes are strongly temperature dependent, they must be treated at finite temperatures. Together with the nonlinear coupling, these three features combine to present a difficult theoretical problem. The thermodynamic, quantum mechanical problem is described by the so-called Takeno Hamiltonian for which no exact solutions exist, although approximate solutions abound with little understanding of their accuracy or range of validity. In some cases the Hamiltonian is truncated so as to preserve quanta in the optical system. This approximation, the so-called Davidov Hamiltonian, omits very important physics from the problem. In other cases a solution is approximated by adopting a product wave function separating acoustic and optic phonon variables. This so-called Davydov Ansatz has been extensively criticized as a serious oversimplification.

In the last year we have brought to bear on these problems the methods of Langevin Equation theory which does not require adopting any of the above approximations, but works directly by calculating the time correlation function $\chi(t)$ of a specified initial excitation from a very large number of moments of the exact spectral density function, obtained in turn from the Hamiltonian equations of motion. Langevin theory proceeds by defining a hierarchy of heat baths $\theta_m(t)$ which interact with $\chi(t)$ and determine how it decays in time. Specifically this year we have accomplished the following:

- (1) Refined a powerful new approach to Langevin theory that makes efficient use of the calculated moments to obtain the spectral density of the first heat bath function $\theta_1(t)$ and thereby calculate the time decay of $\chi(t)$. We have proved that an expansion of $\theta_1(t)$ in a series of newly defined functions $G_k(t)$ critical to the theory is unique and complete.
- (2) We have applied the theory to the problem of a single external oscillator nonlinearly coupled to an acoustic phonon manifold and obtain well converged results for the lifetime and red shift of the external oscillator. In this case the external oscillator frequency lay well within the phonon manifold.

- (3) For this same problem, in the case of the Davydov Hamiltonian, we have obtained an exact solution and found excellent agreement with the Langevin theory solution described above. This has allowed us to verify the valid time domain of the Langevin calculation of $\chi(t)$ and show that it is long enough to obtain accurate results for the time decay of $\chi(t)$.
- (4) We have extended the problem described in (2) above to a parameter regime including a 1000-fold increase in the square of the non-linear coupling constant and an increase in the external oscillator frequency to 16 times greater than the largest frequency in the phonon manifold and continued to find excellent agreement between the exact theory and Langevin Theory.
- (5) We have shown that the Davydov Hamiltonian can be mapped onto a hamiltonian very similar to the Takeno Hamiltonian and therefore has a wider range of application than previously thought.
- (6) We have completed the complex programming required to calculate the moments of the spectral density for the problem of a chain of external oscillators non-linearly coupled to an acoustic phonon manifold. We expect soon therefore to make accurate calculations of the lifetime of localized vibrational states of the kind described above.
- (7) We have nearly completed a first draft of a review paper on the Langevin Equation theory which contains a number of new results important to understanding and applying the theory.

ULTRASONIC STUDIES

Principal Investigator: Robert G. Leisure, Colorado State University
 Ricardo Schwarz, CMS
 Albert Migliori, P-10

One major effort during the visit was an investigation of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ in collaboration with A. Migliori and Z. Fisk. It was of interest to investigate the tetragonal to orthorhombic structural phase transition in this material with as high Sr doping as possible. Unfortunately, it is more difficult to grow single crystals at the higher Sr doping levels. It proved possible, however, with resonant ultrasound to investigate the temperature dependence of the elastic constants with $x \approx 0.18$. The crystal used was extremely small for elastic constant measurements; the total mass was less than 0.5 mg. The expected softening was observed, and the results were used in the formulation of a self-consistent phonon description of the T-O transition. An unusual aspect of the measurements was that the observations were also carried in the orthorhombic phase. A preliminary investigation of anharmonic effects in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ was carried out using resonant ultrasound.

The second major effort during the visit was an investigation of ultrasonic attenuation and elastic constants in rare-earth metal hydrogen systems in collaboration with Ricardo Schwarz and Albert Migliori. Measurements were performed on ScH_x , ScD_x and YD_x to investigate two effects. First, these systems are known to undergo phase transitions near 170K which involve the formation of hydrogen pairs. It is not clear whether the interaction responsible for the phase transition is electronic or elastic in origin. Our measurements showed a change in slope of the elastic constants at the transition: the material is softer below the transition than would be the case if the transition did not occur. Second, both neutron scattering and NMR indicate very rapid hydrogen motion at low temperatures (10K - 100K), although the actual motions are quite different ($10^{11}/\text{s}$ for neutrons and $10^9/\text{s}$ for NMR). It is suspected that tunneling is involved. A rather direct way to investigate tunneling is to look at the isotope dependence. Ultrasound is perhaps uniquely suited for this investigation since it is insensitive to spin. Low temperature attenuation peaks indicated rapid motion in all three materials investigated. A comparison of the results in ScH_x and ScD_x indicated a very large isotope effect. We are currently trying to interpret these results in terms of existing theoretical models.

MANY-BODY CALCULATIONS OF STRONGLY CORRELATED SYSTEMS

Principal Investigator: Lu Sham, University of California, San Diego

Much of my work in Los Alamos has been in collaboration with others. The interaction with members of the Los Alamos Laboratory has been very beneficial to me. In high temperature superconductors, I have had extensive discussions with Al Migliori and Zack Fisk, resulting in collaborative work on the theory of tetragonal to orthorhombic structural phase transitions, which is still ongoing. Mounting evidence on the role of electron-phonon interaction in the superconductivity in the copper oxide superconductors has been acknowledged by even some of the most ardent advocates of the strongly correlated electron mechanism. Study of the electronic effects in lattice vibrations, especially in the complete set of elastic constants which Al and his group can measure accurately for a wide range of temperatures, leads not only directly to the cause for the structural phase transition but also to the possibility of the electron-phonon mechanism for superconductivity.

The collaborative research involving Robert Albers, Matthew Steiner (a graduate student from UCSD supported by INCOR), and myself is entering the third year. The program is the extension of the density-functional theory for the strong correlation in narrow-band electrons metals. The idea is to combine the effects of the onsite Hubbard interaction with the electron interaction effects for far-ranging s and p electrons provided by the local density approximation. From model study which was published before my arrival in Los Alamos, we have moved on to the trial of the idea in the 3d series: iron, cobalt, and nickel. Photoemission spectra have been re-interpreted in our theory in terms of quasi-particle peaks and satellite lines due to onsite interaction. In addition, a broad range of experiments can be explained in a unified manner. Final draft of a paper on this subject is being prepared. We are moving on to the study of a heavy Fermion metal, *raison d'être* from the theory.

As a result of my seminar on the dynamical response of the Fermi sea to interband optical excitation including the hole recoil effects, work done by Uenoyama and myself, Jim Gubernatis, Kevin Bedell and I are exploring the possibility that Monte Carlo computation schemes which has been developed in Los Alamos can be used to solve some of the important outstanding problems in this area. In particular, we want to know if the computational scheme developed by Jim and others for the single impurity many-body effects without hole recoil. The project is just underway. We plan to recruit a graduate student from La Jolla to work on this.

Based on the theory of Uenoyama and Sham on the spin relaxation of holes and electrons in semiconductor quantum wells, I have helped an experimental group AT&T Bell Laboratories in Hilmel to explain these observations in time-resolved luminescence polarization spectra. A surprisingly coherent picture emerges based on our theory. It also points to a number of many-electron effects to be studied. A paper, "Subpicosecond spin relaxation dynamics of excitons and free carriers in GaAs quantum wells," by T. C. Damen, L. Vina, J. E. Cunningham, J. Shah, and L. J. Sham, has been submitted for publication.

ELECTRON STRUCTURE OF FILMS AND LAYERS

Principal Investigator: Samuel B. Trickey, University of Florida

The research during this visit was focused on two primary goals and one secondary one. All of it is in close collaboration with J. C. Boettger of T-1 and more generally is related to those LANL researchers working on first-principles predictions of properties of novel materials at chemical precision levels (e.g. Albers, Boring, LeSar, Mueller, Straub, Wills, et al.).

One major objective was to test, refine, document, and write a User's Guide for the code FILMS. This is a full-potential, all-electron code for treating unsupported ultra thin films with two-dimensional Bloch periodicity and true vacuum boundary conditions in the third Cartesian direction. Boettger and I have been developing and using it for about 8 years and were invited a year ago to publish it, along with a major review article on its algorithmic content, in Computer Physics Communications. A substantial part of my effort while at CMS was devoted to improving code robustness, clarity, and portability and to writing most of the User's Guide; about 80% of my objective was achieved. The main unexpected difficulty was porting to Cray Unicos from other Unix environments (Sun, Convex, FPS, Dec).

The second major objective was to complete several calculations and write the associated papers. Here we succeeded fully. We completely redid the structural energetics of a graphite 2-layer, a system on which I had done a preliminary study earlier. That study had a peculiar c-axis contraction which we had never been able to rationalize; the restudy with much richer basis sets and substantially refined algorithms shows that the contraction was spurious. We finished the structural optimization of Li 1-5 layers and demonstrated a new and dramatic quantum size effect. This is a sharp step in the occupied density of states for each layer. Based on our long-standing interest in the cold-curve of simple metals (as a benchmark for EOS's in general) we wrote a comment on a recent Phys. Rev. B paper pointing out the misleading nature of the calculations and the incorrect physics behind its claimed prediction of the Li solid-solid phase transition.

Finally, as a secondary effort, motivated mostly by Ray Dixon and Fred Mueller, I ported WIEN, my published full-potential LAPW code, to the Unicos Cray (machine R) for use by anyone who might want it.

III. INTERDISCIPLINARY RESEARCH

SURFACE MODIFICATION OF MATERIALS

Principal Investigators: M. Nastasi, MST-7

Introduction

The performance of many materials is controlled by the composition, microstructure, distribution of surface asperities, and presence of defects in the crystal structure near the surface and at interfaces. The ability to control and alter such near-surface features can greatly facilitate the synthesis of novel materials with highly tailored properties. In an attempt to meet the demand for new materials, the processing of novel material configurations with unique microstructure is being explored in systems which are further and further from equilibrium. An emerging class of such materials, which can be synthesized using thin film and ion beam techniques, are alloys and composites with ultrafine microstructures.

Materials modification using thin film techniques such as physical vapor deposition (PVD) or ion beam techniques such as ion implantation, ion beam mixing, and ion beam assisted PVD offer the materials scientist a way to alter both the structure and chemistry of a surface in a highly controlled non-equilibrium manner. The rapid energy dissipation associated with both the PVD and ion beam synthesis techniques can result in the formation of metastable amorphous and nanostructured materials. Ion beam and PVD materials modification research has shown these techniques to have applications in the areas of tribology, corrosion, oxidation, fatigue, superconductivity, optics, and basic metallurgical studies.

The primary thrust of the surface modification research at Los Alamos during the last year has been focused on novel and metastable materials synthesis with an emphasis on oxidation, strength enhancements and improved tribological properties.

OXIDATION

Principal Investigators: M. Nastasi, MST-7
J.R. Tesmer, P-10

Ion implantation has several attributes which distinguish it as a means of oxidation protection. Ion implantation alters only the top few microns of a material, and, unlike traditional forms of alloying, it is unlikely to change bulk properties. We recently examined the effect of yttrium implantation on the oxidation properties of copper, molybdenum and tantalum. Yttrium was chosen for its known ability to produce passive oxides. In addition, Y is immiscible with Mo and Ta making ion implantation the only possible means for alloying. In contrast, Y alloys readily with Cu. The oxidation was monitored using high-energy resonant helium backscattering allowing the surface oxidation to be easily determined without the necessity of weighing samples.

Sample of Cu, Mo, and Ta were implanted over half their surface with 3×10^{16} atoms/cm² at energies chosen to produce a projected range of 350 Å in all materials. Oxidations were made at 200, 400, and 500°C for Cu, Mo, and Ta respectively and for times ranging from 10 min. to 10 h. At short times the oxidation was observed to be enhanced in the Y implanted materials relative to the unimplanted materials. However, as the oxidation time increased the oxidation rate in the implanted materials decreased, and in the case of Cu and Ta the total amount of oxygen in the implanted samples eventually became lower than that of the unimplanted samples. In all cases Y implantation strongly effects the oxidation process. For Ta and Cu retardation of grain boundary oxidation occurs. For Mo, implantation results in the formation of a discrete oxide which appears to grow in a layer-by-layer manner. These experiments indicated that the Y-Cu and Y-Ta oxides are more passivating than their unimplanted counterparts.

TRIBOLOGY

Principal Investigators: M. Nastasi, MST-7
T.G. Zocco, MST-S
T.R. Jervis, CMS

The tribological and surface mechanical properties of metallic and ceramic surfaces have shown marked improvements following ion beam treatments. The bulk of research examining the effects of ion beam processing on the tribological properties of a material have essentially been focused on ion implantation. Early research showed that dual ion implantations of Ti and C into steel produced both increased wear resistance and reduced friction. The improvements resulting from ion implantation alloying have been attributed to the chemical changes and amorphous structure which evolve during the implantation process.

An alternative beam technique which permits high concentration alloying at low ion doses and is capable of producing similar tribological improvements as those observed from ion implantation is ion beam mixing. Recent experiments have examined the properties of metastable Fe-Ti-C alloys produced by the ion beam mixing of a Fe/Ti/C multilayered structure.

A multilayered Fe/Ti/C structure consisting of eleven alternating sublayers, four Fe, four Ti and three C, was ion mixed on a AISI 304 stainless steel substrate with 400 keV Xe⁺⁺. Complete mixing was observed after an irradiation of 1×10^{17} Xe/cm at 550°C (hot). Electron diffraction revealed the formation of the compounds TiC and Fe₃C and a small amount of an amorphous phase. Both compounds possessed an ultrafine microstructure with an average grain size of 45 nm. Some samples were given a second irradiation with 5×10^{15} Xe/cm² at 0°C. The phases present following the second irradiation were ultrafine grained TiC, α-Fe and an amorphous phase.

Both ion processes, hot and hot plus 0°C, resulted in a reduced friction coefficient and improved wear properties relative to untreated stainless steel. However, differences in wear life were observed, with the hot ion mixed sample consistently outlasting the hot plus 0°C treatment. The wear differences are not well correlated with the hardness data which showed both ion process to produce equally hard surfaces. Clearly, surface wear is a complex function of surface mechanical properties and surface chemical interactions at the sliding interface. Since the hardness data indicates that the plastic behavior of the two ion processed surfaces are similar, surface chemistry must be responsible for the wear rate differences observed.

The chemical reactivity at the interface of the sliding system will differ in the two ion beam processed samples due to the different phases present in each. The phase analysis of the hot and the hot plus 0°C ion mixed samples suggest that Fe_3C is less reactive and extends the wear life and/or that $\alpha\text{-Fe}$ is more reactive resulting in a reduced wear life. This hypothesis is consistent with recent tribology data obtained on laser mixed Fe/Ti/C samples which showed that lower friction coefficients and longer wear life were correlated with lower $\alpha\text{-Fe}$ content and a microstructure consisting of fine carbide precipitates and/or an amorphous phase. Thermochemical arguments based on the work of Gerkema and Miedema indicate that the reactivity and adhesion between the 52100 steel pin and $\alpha\text{-Fe}$ will be greater than between the pin and Fe_3C , consistent with the wear life time trend observed.

In short, the difference in wear life in these samples appears to be the result of a difference in adhesive wear which in turn results from differences in the chemical reactivity of the phases formed during ion beam processing.

PVD Synthesized Alloys and Composites with Ultrafine Microstructures

Principal Investigators: M. Nastasi, MST-7
K. H. Hubbard, MST-7
T. R. Jervis, CMS
R. P. Messner, MST-7

Physical vapor deposition and other novel fabrication methods enable materials with ultrafine microstructures either in the monolithic or composite form to be fabricated in a reproducible manner. These materials have been shown to possess strengths which are within a factor of 3 or 4 of the theoretical shear strength $\approx \mu/15$, where μ is the shear modulus. Thus materials with ultrafine microstructures present the opportunity to develop a basic understanding of the deformation and fracture mechanisms which are operating close to the theoretical limit of the strength of materials. The primary goal of this work will be to determine the influence of ultrafine microstructure materials on the properties and mechanical performance of thin film composites composed of advanced materials and to determine the applicability of such materials to improve the mechanical properties of engineering materials composed of brittle ceramics, intermetallics and metals.

In the current program studies involving the performance and synthesis of nanolayered composites have been performed. In one study the role of Fe/Ti nanolayered composite as a tribological coating on tool steel was examined. Nanolayered composites of Fe/Ti were chosen based on previous data in the literature which showed novel alloy surface films of Fe-Ti have been shown to possess good friction and wear properties. These surface alloys have been formed by ion beam techniques such as Ti ion implantation into steels and ion beam mixing of Fe/Ti multilayer on steel substrates, by laser mixing of Ti and steel, and by the coevaporation of Ti and Fe on steel substrates. In all instances the good tribological properties observed in these materials were attributed to the formation of an amorphous phase and/or refined microstructure which evolved during processing. In the present study an as-deposited composite structure composed of 9 alternating layers of 9 nm Fe and 13.5 nm on hardened tool steel was examined for tribological and mechanical properties without any addition processing.

The 90 nm as-deposited nanolayered structure in contact with a 52100 steel ball counter surface possessed a 0.16 friction coefficient and showed good wear character after 1000 cycles in pin-on-disk experiments. Nanoindentation experiments show a 20 % increase in hardness for material in the wear track. Electron microscopy data suggests that the as-deposited bcc-Fe plus hcp-Ti multilayer composite transforms to a nanocrystalline alloy of unknown crystal structure with a dispersion of nanocrystalline bcc-Fe. Apparently this alloying resulted from a solid state reaction induced during pin-on-disk friction and wear test. The low friction and increased hardness observed in these surface films is attributed to the formation of nanocrystalline dispersion strengthened composite structure.

Addition experiments involving the mechanical properties and stability of Cu/TiB₂ nanolayer structures have been also performed. Current research activities involves the synthesis and mechanical property evaluation of α -Al₂O₃/RuAl, W/Cu and B/Cu nanolayered composites.

LASER SURFACE PROCESSING

Principal Investigators: T. R. Jervis, DIR-ESD
 J-P. Hirvonen, MST-7
 M. Nastasi, MST-7
 K. Hubbard, MST-7 (postdoc)
 T. G. Zocco, MST-5
 J. H. Steele, NMT-5
 J. Ruud, Harvard University
 Scott Barnett, Northwestern University
 Anna Zurek, MST-5
 J. Petrovic, MST-4
 A. Bhattacharya, MST-4 (postdoc)
 Li Luo, CMS (postdoc)

RESULTS:

Summary:

Direct efforts in this program during FY 1991 concentrated on two systems; excimer laser surface processing of Ti-6Al-4V, and excimer laser mixing of Ti on Si₃N₄. In each case the relationships among process variables, microstructure and composition, and properties were examined. In addition to these direct efforts, a number of collaborations continued, some of which were in support of programmatic efforts. A particularly gratifying event was the recognition of our laser mixing work by news articles in *Nature* and *Materials Edge*.

Laser Surface Processing:

Work in the previous year on the properties of excimer laser processed Ti-6Al-4V, including laser heat treating, laser melting and solidification, and B alloying of the surface suggested that oxygen incorporation was occurring during laser processing. Questions remaining about the effect of the initial surface treatment (mechanical polish vs. electropolish vs. as rolled) led us to continue our experiments only with electropolished surfaces, as these are as strain free as possible. By treating the surface with multiple overlapping laser pulses, up to 60, we found that we formed a uniformly fine-grained surface of TiO. The evolution of this surface phase proceeded directly from the martensite which is the result of quenching from the initial laser pulse to a mixed phase of the martensite and TiO, to a nearly pure TiO surface layer. Of particular interest was the absence of an intermediate Ti₂O phase and a final TiO₂ phase, both of which would be expected in an equilibrium oxidation process. Ion beam measurements of the O:Ti ratio as a function of depth, performed by K. Hubbard, showed that beyond a certain point, approximately 45 pulses, further oxygen incorporation resulted only in a thicker TiO layer. Nanoindenter measurements of the processed surfaces show that the dependence of the hardness varies in a systematic way with oxygen concentration. This dependence is still under study and will be reported in the coming year. We also hope to investigate the tribological properties of this surface phase; solid-lubricated light-alloy gears and bearing being of great interest for applications in space. The B alloying experiments, while of interest in producing a surface alloy with an amorphous microstructure, did not yield interesting surface mechanical properties so this avenue was discontinued. Kevin Hubbard, Mike Nastasi, Jim Steele, and Tom Zocco are involved in this work.

Another series of experiments, also begun in the previous year, was on process-property relations in surface alloyed Si₃N₄. Our earlier work on SiC showed that

substantial improvements in tribological properties were available through surface alloying with Ti. This work and that of Narayan at NC State further suggests that improvements in bulk fracture strength of ceramics can be obtained from this process. Because one of the most promising materials for tribological applications is Si_3N_4 , we decided to expand our alloying experiments to this material. Initial experiments had not been promising. Some mixing occurred; Si was found to diffuse into the Ti, but the mixing was not complete. We presumed that formation of TiN at the interface between the Ti and the Si_3N_4 presented a barrier to further mixing. A series of experiments at higher incident fluences, which produce much higher temperatures in the surface layer, resulted in complete mixing, both of thin layers (100 nm) and much thicker ones (400 nm). These latter resulted in mixed layers, with a broadly graded interface to the substrate, of almost a micron in thickness. As in the surface modified Ti case, we expect to investigate the surface mechanical and tribological properties of these materials in the coming year. Mike Nastasi, Juha-Pekka Hirvonen, and Kevin Hubbard are involved in this ongoing work.

Collaborations:

As in prior years, much of our work has been done in collaboration with others, both in basic research areas and in support of programmatic efforts. A collaboration with Jim Ruud (Harvard Univ.) and another with Scott Barnett (Northwestern Univ.) both are directed towards examining the hardness and elastic modulus of nanometer scale multilayer structures using the nanoindenter. Kevin Hubbard has been the principal investigator working with the Northwestern group. Ruud's work involved multilayers of Ag and Ni, while the Northwestern work was on single crystal multilayers of TiN and (V-Nb)N. The essential result of these measurements is that the effect of multilayer repeat length is the same in the metal-alloy and single-crystal cases, that there is an effect of repeat length on the hardness, but that there is no evidence for a "supermodulus effect."

A number of experiments on laser mixing of Ni/Si/SiO₂/Si were made in collaboration with Li Luo. The laser mixing experiments, in conjunction with furnace annealing, were intended to form single crystal NiSi₂ on SiO₂ on Si. The results were somewhat inconclusive, and this work is not continuing. Nanoindenter experiments of hardness on adiabatic shear bands, in support of programmatic work by Anna Zurek, showed general agreement with previously published results. However, an expected abrupt (on a scale of μm) increase in the hardness at the shear band was not observed. Finally, several sets of nanoindenter measurements were made for Arun Bhattacharya and John Petrovic in support of their OBES programmatic work. Indents were made in a series across the interface between single crystal SiC whiskers and a hot pressed Si_3N_4 matrix. Although the Si_3N_4 was expected to be rather hard, this turned out not to be the case.

DEVICE APPLICATIONS IN LOW-DIMENSIONAL MIXED-VALENCE SOLIDS AND THIN FILMS

Principal Investigators: B. I. Swanson, INC-4
A. R. Bishop, T-11

This work is part of a larger project on novel low-dimensional electronic materials. The materials of interest are inorganic polymers consisting of alternating transition metal complexes and bridging groups that form linear chains in crystalline solids (MX and MMX solids). The electron-electron and electron-phonon (e-e and e-p) coupling is extremely strong down the chain axis with relatively weak inter-chain coupling. The symmetric structure with the halide ions equidistant from the neighboring transition metal complexes is unstable with respect to a Peierls distortion and a commensurate charge transfer between metal ions to form a charge-density-wave (CDW) along the chain axis in the ground state structures of most of these materials. These solids represent a large tunable class of materials where the ground state structures can be varied from strong to weak CDW (i.e., PtCl-PtI) and, in the case of NiBr and Pt₂Br under pressure, a spin-density-wave (SDW) state.

The current program includes efforts in theoretical modeling, physical characterization, and novel new materials with optimal properties as well as the preparation of a coherent set of materials for which the ground state properties are tuned among differing broken symmetry states. The goal of the efforts on characterization and theory are to derive a detailed understanding of the physical properties of this class of materials as the ground states are tuned into the phase boundary region between CDW, SDW, and conducting states. In addition to characterization and modeling of the ground state properties as the e-e and e-p forces are tuned, this task involves developing a detailed microscopic level understanding of local gap states (polarons, bipolarons, excitons, and kinks). The focus of the work that is now supported by the CMS is the extension span nonlinear optics (as per MX solids and related thin films), heterojunction materials for nonlinear optics and energy storage and conversion (the mixed metal and mixed halide MX solids), and chemical sensors (covalently bonded self-assembled monolayers and multilayers).

The experimental aspects (BIS) of the CMS supported research is focused on preparing self-assembled monolayers and multilayers of transition metal complexes on oxide surfaces. (Research of the mixed halide and mixed metal solids and heterojunctions is supported by other funds.) The original intent was to prepare mixed-valence chains (much like the chains in the MX solids) that are covalently bonded to oxide surfaced one layer at a time so as to control the orientation of the charge transfer dipole for nonlinear optical (NLO) materials applications. The novel aspect of such self-assembled multilayers of mixed-valence dimers is the potential for tuning the intervalence charge transfer (IVCT) absorption band to optimize second harmonic generation of the thin film. For virtually all NLO materials now used for second harmonic generation, the absorption bands are well to the blue of the second harmonic signal thereby giving rise to very different dielectric properties for the fundamental and the harmonic. If the charge transfer absorption can be tuned to be intermediate with respect to the fundamental and the first harmonic, the phase matching problems inherent in second harmonic generation can be obviated.

The chemical approach for covalent bonding of transition metal complexes directly to oxide surfaces is to rely on O-Si-R (where R- a multidentate ligand) linkages to couple the first transition metal complex to the surface. The metal complex is then modified to accommodate a bidentate ligand capable of bridging between the first and the second metal complex. This process can then be repeated to build multilayers of metal complexes on the

surface. We have explored two different types of metal complexes during this year. The first is a $\text{Ru}^{\text{II}}/\text{Ru}^{\text{III}}$ dimer where a five coordinate ligands is used to bind Ru^{II} and pyrazine is then used to bridge to a Ru^{II} complex. The second system is 5, 10, 15, 20-Tetra(4-pyridyl)-21H, 23H-porphine superlattices. Both systems have been characterized by optical absorption, FTIR-ATR spectroscopy, X-ray photoelectron spectroscopy, secondary ion mass spectroscopy, and ellipsometry.

Second harmonic generation (SHG) was carried out at the Nd-YAG laser fundamental ($1.06\ \mu\text{m}$) and we found that the second order nonlinear optical properties of the porphine derivatives are enhanced due to completely delocalized π -electrons. A theoretical fitting was performed and the average molecular orientation was determined via polarization selected SHG measurements in transmission.

The potential application of the covalently bonded self-assembled monolayers and multilayers for developing species selective chemical sensors has also been explored. By monitoring the change in the intrinsic optical absorption properties upon bonding/association/complexing, we have developed a chemical sensor based on the perturbations of incoming guest species to the host system. Preliminary studies of the interaction of organo halides, which are important target toxins within the DOE and the DoD, with the porphine system show promise. At slightly elevated temperatures, the pyridyl groups on the porphine ring were quaternized by methyl iodide and this reaction destroy the charge transfer features of the porphine covalently bonded self-assembled monolayer with a concomitant change in the optical absorption from 447. to 437 nm. The Ru^{II} monolayer also shows promise for the development of a reversible chemical sensor for selected organic toxins such as pyridine and acetonitrile. Work is underway to further characterize the interaction of the Ru^{II} monolayers with organics and the potential for reversible electrochemical sensors developed around this type of complexation.

In the theoretical aspects of this work, we have now achieved a successful calibration of single crystal MX materials as a class with our 2-band extended Peierls Hubbard many-body model -- successful prediction of ground state and polaronic doping state properties. Including dimerization, optical gap, infrared and Raman frequencies, and ESR. This success has allowed us to quantitatively predict properties of mixed-halides, including electronic and phonon signatures for edges, segment lengths and photodecay channels. We are, therefore, now poised to use this modeling to help design prototype device configurations and geometries and we have spent the last year beginning to put this capability into place. In particular, we have developed the theoretical base to model: (a) heterojunctions (periodic arrays of mixed halide MX units) and homojunctions (periodically doped single halide MX chains) for electrooptic, magneto optic, and charge storage applications; (b) dielectric properties in the microwave region; and (c) nonlinear optical properties. We have begun modeling the origin and mechanism of relatively large 3rd-order optical susceptibilities recently reported in MX materials. In particular the process of 2-photon absorption and third-harmonic generation. Our aim is to understand electrooptic and magneto optic responses for specific potential applications such as optical switching devices, nonlinear directional couplers and microwave integrated circuits. We are also poised to model SHG for the covalently bonded monolayers and multilayers that have recently been synthesized and characterized as part of this extension of the low-dimensional mixed-valence solids program.

X-RAY ABSORPTION SPECTROSCOPY STUDIES OF HIGH- T_c SUPERCONDUCTORS

Principal Investigators:

I. Raistrick, MEE-11
S. Conradson, MEE-11
J. Mustre de Leon, MEE-11
A. Bishop T-11

Background

In our original sets of experiments we first discovered the existence of axial-oxygen lattice instabilities in high-temperature superconductors. Although the microscopic origin of superconductivity in copper-oxide-based materials is still a matter of debate, several experiments have now confirmed the existence of structural instabilities and anomalies in the phonon spectra in these materials, suggesting the importance of phonons in connection with the superconductivity mechanism. Accordingly, we have shifted the emphasis of our experimental studies from the original characterization of lattice anomalies in $\text{YBa}_2\text{Cu}_3\text{O}_7$, to other copper-oxide based superconductors. A systematic study of these instabilities as a function of composition and T_c will allow us to discriminate at a quantitative level different theories which predict anharmonicity and lattice instabilities in these materials.

Several experimental techniques based on local probes are now used to investigate the presence of lattice instabilities. Among these techniques are ion channeling, ultrasound resonance, optical spectroscopies, i.e., Raman and infrared spectroscopies, neutron scattering, including pair-distribution function analysis, and x-ray absorption fine structure spectroscopy. In order to gain insight on the fundamental nature of these instabilities, it is important to correlate the results obtained using these different techniques. Thus, we have proceeded with a theoretical effort with emphasis on presenting an underlying mechanism that correlates the results obtained using different techniques and which might explain the microscopic mechanism for superconductivity in the copper-oxide materials.

The recent resurgence of emphasis on the role of phonons in high-temperature superconductors, to which our findings have contributed, has been reflected in the content of the high-temperature superconductivity sessions at the March 1991 meeting of the American Physical Society and other international meetings in high-temperature superconductivity. This has culminated in our involvement in the organization of a workshop on Lattice Effects in High- T_c Superconductors (January, 1992) in conjunction with the University of Pennsylvania and Boston University, supported by CMS and ERDC.

We feel that the highly successful outcome of this project has been the result of a close collaboration between experimentalists and theorists. Rigorous quantitative analysis of important experimental findings has resulted in the formulation of concrete theoretical models which explain in a unified manner several experimental observations in these materials. These models in turn, have suggested new directions for the experimental efforts.

Experimental Studies

We have extended our original x-ray absorption fine structure (XAFS) studies on the temperature dependence of the $\text{Cu}(1)\text{-O}(4)$ radial distribution function (RDF) across the superconducting transition to the dependence of this RDF on stoichiometry and thus T_c . To this end, we have determined the Cu-O RDF's in $\text{YBa}_2\text{Cu}_3\text{O}_7$, $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$, and $\text{YBa}_2\text{Cu}_2\text{O}_{7+d}$ from the Cu K-edge polarized XAFS, using model potentials to

describe the effect of the Cu-O relative motion. In all cases we found that the axial oxygen atom moves in a double-well potential, while in contrast we found no evidence for in-plane anharmonicity of the Cu-O in-plane bonds. Although we have only studied three systems, we were able to establish a qualitative correlation between anharmonicity of the Cu(1)-O(4) bond and T_c —specifically, the higher T_c the higher the tunnelling rate between the two Cu-O(4) sites. This result was published as a rapid communication on Physical Review B in August 1, 1991.

We have also analyzed the Cu K-edge XAFS of $Tl_1Ba_2Ca_3Cu_4O_{11}$ as a function of temperature. As in $YBa_2Cu_3O_7$ we have found two axial-oxygen positions in this material; However the analysis shows that the changes in the two axial-oxygen positions, across the superconducting transition, are larger than in $YBa_2Cu_3O_7$. This study showed that lattice fluctuations are present in other high-temperature superconductors besides $YBa_2Cu_3O_7$, and pointed to a correlation between anharmonicity and T_c . In addition, it shows a stronger coupling between the ionic motion and superconductivity as T_c increases. As in $YBa_2Cu_3O_7$ we explained these results, in a qualitative way, as resulting from charge transfer between Tl-O and Cu-O planes, reflected in the motion of the axial oxygen connecting these planes. This study will appear in the November 1991 issue of Physical Review B.

We have initiated a collaboration with Dr. M. Subramanian of Dupont on the study of $Tl_1Ba_{2-x}Sr_xCuO_6$. In this material, as the Sr concentration is varied, T_c changes from 0 to 90 K, with only small effects on the local structure of the Cu-O and Tl-O planes. Consequently, the analysis of these materials should allow a more straightforward connection between charge transfer (between these planes) and the axial oxygen dynamics. We have collected data as a function of temperature for 6 different Sr concentrations at both the Cu K- and Tl L_{III} - edges. The analysis of these data will provide a detailed quantitative correlation between the axial-oxygen lattice instability and T_c . These data will also allow us to study the bonding in the Cu-O planes which, in the case of $YBa_2Cu_3O_7$ was made difficult by the presence of Cu-O chains.

Finally, in collaboration with Prof. T. Egami from the University of Pennsylvania, we are studying the Cu K- and Tl L_{III} - edges XAFS of $Tl_2Ba_2CaCu_2O_8$. Prof. Egami's pair distribution analysis of neutron diffraction data in this system indicates the presence of two axial oxygen positions as well as changes in the structure of the Cu-O planes across the superconducting transition. Theoretical models which lead to two axial oxygen positions indicate that the separations between the axial oxygen positions measured using XAFS and pair distribution analysis of inelastic neutron scattering should be different. Consequently a comparative study of the XAFS and neutron scattering data will provide tests of the validity of different theories which predict the observed double-well behavior.

Theoretical Studies

We have discussed the implications of the observation of a split Cu-O(4) position using XAFS in diffraction experiments. We have concluded that if there are dynamical oscillations between the two axial-oxygen positions, as implied by the XAFS experiments, these two positions will not be observed in conventional diffraction experiments. This prediction is in agreement with recent comparisons between pair-distribution analysis of inelastic and elastic neutron diffraction experiments by the University of Pennsylvania group. This study highlights the complementarity of diffraction studies and XAFS. Diffraction provides an accurate determination of the static structure of a compound, e.g., interatomic distances and coordination numbers; XAFS uses this information in order to

study more subtle aspects of the pair-distribution functions. This result and a detailed account of the theory developed to analyze the XAFS experiments will appear in Physical Review B, December 1, 1991.

We have performed an exact diagonalization of a Peirls-Hubbard electron-phonon Hamiltonian, originally proposed by A. Bishop, for the $O(4)-Cu(1)-O(4)$ cluster in $YBa_2Cu_3O_7$. We consider a linear electron-phonon coupling for infrared and Raman active phonons in this cluster. For large enough electron-infrared phonon coupling, the motion of holes and ions becomes strongly correlated, *i.e.*, polaronic, leading to a double-well structure for the infrared mode, as that encountered in the XAFS experiments. In contrast, the associated Raman mode shows a single-well behavior even for large electron-Raman phonon coupling. This model leads to a unified description of structural and optical observations for the axial oxygen in $YBa_2Cu_3O_7$. It also shows an underlying polaronic origin for the two-well structure observed in XAFS and other experiments, demonstrating the presence of holes at the axial oxygen site. This last prediction has been corroborated by near-edge x-ray absorption studies by other groups. The appearance of polarons in this model is accompanied by nonadiabatic behavior indicating that, although anharmonic lattice dynamics models can describe in an adequate form structural results, they lead to optical spectroscopic predictions inconsistent with experiment. We are currently studying the nature of excited states in this model which should allow us to make quantitative predictions for the optical spectroscopy. A manuscript containing these results has been submitted to Physical Review Letters on October 1991.

We plan to extend this model in order to include electronic and phononic degrees of freedom in the Cu-O planes. This should result in a characterization of the spatial extent of the observed polaronic distortions, and their effect in the pairing mechanisms of holes in the planes.

SUMMARY OF RESULTS ON LAMPF EXPERIMENT 1235 MUON LEVEL CROSSING RESONANCE SPECTROSCOPY

Principal Investigators: D. W. Cooke
M. Leon
M. A. Paciotti

PARTICIPANTS: C. Boekema (San Jose State), J. Brewer (U.B.C.), S. F. J. Cox (RAL), E. Davis (U. Leicester), T. L. Estle, B. Hitti (Rice), R. Kiefl (U.B.C), J. Lam (San Jose State), D. Lamp, R. Lichti (Texas Tech), A. Morrobel-Sosa (Cal. State S.L.O.), J. Oostens (U. Cinn.), J. Schneider (TRIUMF)

Muon level-crossing resonance spectroscopy (μ LCR) has been established as a powerful variant of μ SR as a tool in materials science. The integral μ^+ decay asymmetry shows dips as a function of longitudinal magnetic field because of cross relaxation, when the muon Zeeman splitting coincides with the energy splitting of a neighboring nucleus. Measuring this dependence gives valuable information on muon stopping sites and hyperfine interactions in metals, semiconductors, insulators, high temperature superconductors, and organic compounds. Because it is an integral technique, the full LAMPF μ^+ intensity can be used with essentially no penalty for the duty factor -- in extreme contrast to the more standard time-differential μ SR, which allows only a single μ^+ in the target during an $\approx 20 \mu$ s time interval.

The 9 days of beam time used in June/July were devoted to beam development, controlling background, measuring asymmetry (see Fig. 1), and especially to studying the stability of the positron (e^+) signals. After cuts were made to eliminate data from interrupted beam, short macropulses, etc., the ratios of positron detector counts were found to be remarkably free of systematic drifts. (This is emphatically not the case at TRIUMF and RAL). An alternating "flip field" with subtraction are needed at TRIUMF to detect a change in asymmetry. Fig. 2 shows the results of ramping over a field interval many times (40 min. $\times$ 45 cpm). The deviation of the ratio from its average is plotted in units of the expected statistical standard deviation (here 6×10^{-4}); no variation outside of statistics is visible, so this kind of averaging appears to be entirely adequate in picking out a small dip in asymmetry as a function of field. Thus, it appears that LAMPF can indeed be a leading facility for μ LCR.

The early LAMPF shutdown prompted by DOE Tiger Team preparations allowed only 6 days of beam time in August for μ LCR experiments. During this time we investigated effects of large counting rates on μ LCR spectra, and studied possible ways to minimize the effects. Beam development studies culminated in measuring the μ LCR spectrum of single-crystal copper. The resonance occurs at 77 Oe with FWHM of 24.7 Oe, and is easily resolvable as shown in Fig. 3. These results demonstrate that LAMPF is a prime facility at which μ LCR can be performed. Moreover, given the high muon flux, with corresponding high data rate, LAMPF should be considered a world-class μ LCR facility.

IV. ADVANCED STUDIES PROGRAM

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This program was started in 1988 as a joint program between the Laboratory and Public Service Company of New Mexico called "Advanced Studies Program in High-Temperature Superconductivity Theory" dedicated to advancing the development of the theory of these new and exciting materials. The program was built around a group of external scientists called "PNM Fellows" led by J. Robert Schrieffer (UC Santa Barbara). The other PNM Fellows were Elihu Abrahams (Rutgers University), Maurice Rice (ETH, Zurich), David Pines (University of Illinois), and Sebastian Doniach (Stanford University). With the withdrawal of PNM due to financial problems in 1989 it was decided to develop this into a Laboratory LDRD funded program. This was successful and this is the second year of the restructured program.

This new program is built on a triad of three elements: the Los Alamos experimental effort coordinated by ERDC, the T-Division theoretical effort (both microscopic and phenomenological), and significant consultant interaction with leading theorists throughout the world (developed in the PNM program). The Fellows program consists of five scientists lead by J. Robert Schrieffer who is the Director of the program. He is joined by David Pines, Elihu Abrahams, Sebastian Doniach, and Maurice Rice. Each scientist spends 20 to 40 days at Los Alamos working on the program. Other scientists are brought to Los Alamos to work with the Fellows and with Los Alamos staff to add breadth to the program and to focus on specific scientific issues. Kevin Bedell of group T-11 is the Deputy Director of the program and in that role acts as the technical coordinator.

One of the most important elements of the program is the postdoctoral fellows in that they have coupled well with the Laboratory staff and have carried out collaborative research with the senior fellows and Laboratory staff. There have been several postdoctoral fellows in the program starting with Arno Kampf from Germany, who left last year to work for a year at UC Santa Barbara. Dermot Coffey from Ireland was the second postdoctoral fellow and he will leave the program this year. He is joined by Masahiko Inui from Japan and Alexander Balatsky from Russia. All the postdoctoral fellows have had strong collaborations with the fellows and Los Alamos staff leading to several co-authored publications.

The program structure includes an emphasis on strong working level scientific interactions between the Los Alamos and external participants. This functions as a method of communicating and integrating theoretical and experimental results and concepts so that progress towards an understanding of these new materials is enhanced.

Structured activities are also a part of the program. In August, a two week intensive study period is held when all the consultant scientists are at Los Alamos. They, with Los Alamos staff and selected visitors, focus on specific scientific issues that theoretical and experimental programs must address.

However, the major activity of the ASP this year was the "Phenomenology and Application of High Temperature Superconductors, 1991" held August 22-24, 1991 in Los Alamos. This was the second such symposium, the first being "High Temperature Superconductivity: The Los Alamos Symposium 1989" held in December, also at Los Alamos.

The idea for these Symposia came in discussions among the organizers on ways in which the ASP might be able to improve communication among researchers on high temperature superconductivity. The problem is not that there are too few international conferences, it is that there are so many with a plethora of invited and contributed papers, and too little time for informal discussion. They therefore were led to look back to a

different time in physics, when it was possible to gather, in one not-too-large room, a group of leaders in a sub-field under circumstances which encourage both reflection and extended informal discussion.

The Solvay Congresses of the period 1927-1955 provide a paradigm for the sort of conference we hoped might be useful: some 30-40 participants in a meeting organized around a program of a small number of comparatively long (1 1/2 hour) talks by invited rapporteurs, followed in each case, by a long period devoted to informal discussion and a few brief research reports. It was believed that such a symposium would be highly beneficial to the participants, but that for it to have impact on the wider scientific community it would be necessary to publish proceedings, including a detailed account of the informal discussion following each report, and to publish these promptly.

The first Symposium dealt with microscopic mechanisms in these superconductors and covered topics such as experimental data summary, normal state properties, and various theoretical models of the superconducting state. The second Symposium was held to treat topics such as microwave properties, Josephson Junctions, vortex behavior, and a survey of applications. In both symposia each session began with a long talk by a rapporteur who has critically reviewed the topic in question and continued with extensive discussion of that topic.

The proceedings of the first Symposium were published in near-record time by Addison-Wesley. This has been a very successful book with over 800 copies sold in the first year with very little advertising. (This was, in fact, a best seller for Addison-Wesley last year.) This Symposium has had an impact on the whole scientific community working on high T_c superconductors in redirecting attention to the metallic character of the materials and the normal state properties. The second book will also be published in near-second time by Addison-Wesley and should be out in December 1991.

Although this program is only in its second year of LDRD funding we have decided roll this program over into a new program that broadens the interest from a tight focus on High T_c Superconductivity to a Program in Correlated Electron Theory (PCET). The theme of this new program will be the theory of strongly correlated electronic systems such as heavy-fermion, metal-insulator transition, quantum hall effect systems and similar systems.

The PCET is designed to bring together the program fellows, Los Alamos staff and the University of California (UC) with a focus on correlated electron systems. At Los Alamos we have internal support (LDRD) and DOE-OBES support for theoretical research in correlated electron systems. We are also currently working on redirecting funds from a collaborative research project (INCOR) on HTS with the University of California to a correlated electron theory program. The programs funded through the CMS and INCOR will be used to bring the fellows, visitors, and UC faculty and students together with Los Alamos staff to carry out collaborative research on correlated electron materials. The central research activity will be focused around the month of August. The UC faculty and students are expected to be here during this month. What we would like to see grow out of this program are several ongoing research projects. The ideal project would involve one of the fellows, a Los Alamos staff member or postdoc, a UC faculty member, and a student.

The people associated with the new program are:

Director: Kevin Bedell (T-11, Los Alamos)

Fellows: (The following are the names of the individuals who have agreed to become fellows.)

Professor Elihu Abrahams (Rutgers)

Professor David Pines (University of Illinois)

Professor Douglas Scalapino (UC Santa Barbara)

Professor J. Robert Schrieffer (UC Santa Barbara)

Professor John Wilkins (Ohio State University)

Postdocs and Long Term Visitors: Currently in the program

Dr. Alexander Balatsky (JRO CMS, Los Alamos)

Dr. Dermot Coffey (Visitor/Collaborator CMS, Los Alamos)

Dr. Masahiko Inui (Postdoc CMS, Los Alamos)

V. NATIONAL HIGH MAGNETIC FIELD LABORATORY

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The National High Magnetic Field Laboratory program funded by the NSF is a joint program between Florida State University, University of Florida, and Los Alamos. Don Parkin, CMS Director, is one of the three principal investigators on the NSF proposal. The local program is managed by the CMS with the programmatic activities being carried out in M-6 and MST-6.

Funding was received from NSF through FSU in March 1991, at which time the program was formally started. The focus of the Los Alamos element is to develop the high field pulsed magnet program. Both magnet design and development and magnet materials development programs were started this year. During FY92 the program will move forward to provide user facilities including explosive flux compression based 100T and 200T systems, a 20T superconducting magnet station, and a 50T 5ms pulsed magnet station. The magnet stations will be supported with instrumentation and dilution refrigerators.

This is an exciting program in materials science and basic research that brings national and international visibility and recognition to Los Alamos. It also provides unique program development opportunities. The CMS involvement in and management of the NHMFL program is part of its development of the Los Alamos materials science community.

VI. SUMMER RESEARCH GROUP

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The CMS Summer Research Group in Materials Science composed of David Embury, Michael Ashby, David Clarke, John Hirth, John Hutchinson, and Frans Spaepen met for two week session between August 5-16, 1991.

The group started its activities with a four day workshop on "Process Modelling in Materials" which was organized by Fred Kocks and Mike Ashby. This meeting, which focused on many aspects of process modelling, had about 90 attendees, and several nationally known speakers. The talks focused on:

- Criteria for successful modelling, post-evaluation and validation
- Modelling methodologies
- Case studies of successful (and unsuccessful) modelling
- Analytical Modelling versus Simulation
- Needs and opportunities for modelling
- The problem of acquiring data for and from models
- Computing opportunities

The emphasis was on modelling of complex macroscopic processes in which several "unit" processes operate in parallel or in series. The breadth of process modelling issues covered can be seen in the meeting agenda given in Appendix C. The workshop was followed the next week by many informal discussion between the SRG and Los Alamos researchers to outline opportunities in process modelling. This was followed by a discussion between members of the SRG, Los Alamos Staff, and the Laboratory Director on the possibility of creating a Center for Materials Modelling at Los Alamos.

VII. VISITORS PROGRAM

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The visitors program plays a major role in stimulating interaction on important materials science issues among scientists at Los Alamos and outside scientists. During this period the CMS sponsored visitors at the request of researchers from LANSCE, CLS, T, INC, EES, MST, NMT, P, MEE, and CMS. Generally, these visits were for a few days to a week duration. However, twenty of the 143 visitors were at Los Alamos for several weeks and another thirteen were here for one to six months. Our long term visitors included Sam Trickey (University of Florida), who was here from January through May 1990. Sam worked with staff members of T-1 on developing methods for performing multilayer electronic structure determinations. Another long term visitor was Bob Leisure (Colorado State University), who was here from October 1990 through April 1991. Bob worked with both Ricardo Schwarz and Al Migloire (P-10) on ultrasound techniques and measurements. Another long term visitor was Jon Lawrence of UC-Irvine who worked with Joe Thompson (P-10) on crystal growth and characterization. Many of the visitors broaden their interaction with the staff by presenting a seminar as part of the CMS Seminar Series. This year some 32 such seminars were presented. The Condensed Matter and Materials Colloquium enjoyed another successful year with some 30 lectures. The wide variety of topics is indicated by the lecture titles. The complete list of seminars and visitors is given in Appendices A and B.

VIII. WORKSHOPS

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During this reporting period the CMS held nine workshops. The detailed of these workshops listed below can be found in Appendix C. From this list one sees the wide variety of diverse communities served by these workshops. The Los Alamos development of the pulsed field techniques for the National High Magnetic Field Laboratory in conjunction with the Florida State Universities prompted two meetings. The first, held in November 1990, focused on materials aspects of magnetic designs. The second, held in September 1991, focused issues of concern in developing Long Pulsed Magnets. Our Advisory Committee workshop was a review of some of the existing CMS program along with a discussion of possible new research directors. In February, we held a workshop on the dynamics of Microstructures in Materials. This was an attempt to bring condensed matter physicists and materials scientists together to develop a common view of materials problems such as failure and deformation. The annual OBES Materials Science Information and Review Meeting was held at Los Alamos in May. this meeting gives Los Alamos and Sandia researchers an opportunity to present their progress on various BES programs at each lab. The INCOR meeting in April enabled us to bring together all the UC-Los Alamos collaborators in materials research. This was very beneficial because it demonstrated the breath and strength of this program and will probably lead to new collaborations. The "Forum on Ion Beam Analysis" workshops was the framework for a book to be published on Ion Beam Analysis sometime next year. The four day workshop on "Process Modelling in Materials" organized by the Summer Research Group was very important in developing the ground work for a larger materials modelling effort at Los Alamos. Finally, the "Phenomenology and Applications of High Temperature Superconductors, The Los Alamos Symposium: 1991" was as much of a success as the first solvay-like symposium held in 1989. The proceeding of this symposium like the first one will be published by Addison-Wesley.

List of Workshops

National High Magnetic Field Laboratory: Magnet Design Workshop
November 5-6, 1990

External Advisory Committee Meeting
December 10-11, 1990

Dynamics of Microstructures Workshop
February 25-27, 1991

Materials Sciences Information and Review Meeting
May 20-30, 1991

INCOR Meeting
April 26, 1991

Process Modelling in Materials
August 5-8, 1991

Forum on ion Beam Analysis
August 8-10, 1991

Phenomenology and Applications of High Temperature Superconductors, The Los Alamos Symposium: 1991
August 22-24, 1991

National High Magnetic Field Laboratory: Workshop on Long Pulse Magnets
September 30 - October 1, 1991

IX. CMS FACILITIES

IX. CMS FACILITIES

A. GENERAL FACILITIES

CMS Office Facilities

In May of 1985, the CMS moved into a new 4600 ft² office addition to SM-32. The building provides space for the CMS administration, members, visitors, and has an excellent seminar room. The facility has played a large role in the development of the intellectual community surrounding the CMS. In addition, the seminar room has become a very popular place for talks and meetings for the entire Laboratory.

CMS Office Transportables

The growth of the CMS visitor program and the need to assist Laboratory staff with space in the CMS complex exceeds the available space. A 28' x 60' office transportable was purchased and installed immediately east of the present CMS complex. This space has seven two-person offices and one large multiperson office. Over the last four years we have added four more trailers and this combined space houses about forty researchers from either CMS or Laboratory Divisions. We have again reached capacity and are in need of more office space.

B. SCIENTIFIC FACILITIES

Ion Beam Materials Laboratory

The Ion Beam Materials Laboratory (IBML) is a resource for materials related research which provides a core support laboratory for the use of ions to modify and analyze materials. The IBML has completed its third year with both the ion implanter and tandem accelerator fully operational. Four of the five planned beam lines and capabilities are:

- 1) **General purpose:** Routine backscattering and nuclear reaction analysis. 5-axis goniometer for channeling. Elastic recoil detection of H and He.
- 2) **Single Event Upset:** Transient response of electronic devices to charged particle transit. Activation analysis of materials.
- 3) **Ultra High Vacuum:** Dual UHV chamber system with sample transfer between surface analysis (XPS, Auger, ISS, TDS, etc.) and ion analysis.
- 4) **Nuclear Microprobe:** Spatially resolved X-ray, backscattering, and nuclear reaction analysis of materials.

The one remaining combined implanter/tandem beam line, which will have temperature controlled goniometer stage and energy dispersive X-ray diffraction, is in construction.

Both the implanter and the tandem accelerator have been fully operational throughout the year. The tandem accelerator has proved to be highly reliable providing over 2000

hours of beam time. There were only two unscheduled 1-day tank openings. The ion implanter operated approximately 500 hours.

The major users of the laboratory are divisional staff (MST, MEE, P, INC, EES, CLS, WX), ERDC, and external collaborators. Over one-third of the use of this facility was by Post-Docs and University faculty. Significant experimental efforts are in progress in the areas of high temperature superconductors, single event upsets in semiconductor devices, surface modification of materials by ion implantation and mixing, trace element analysis in geologic materials, hydrogen and helium behavior in materials, and characterization of electronic materials.

Electron Microscopy Laboratory

The electron microscopy laboratory is a highly effective CMS user facility serving both the Laboratory staff and outside collaborators. Over one-half of the use of the facility is by Post-Docs and University faculty. The present array of microscopes includes the two new Philips CM30 (300 kV) transmission electron microscopy (TEM), and a Cam Scan Series 4 scanning electron microscopy (SEM). The SEM has x-ray energy dispersive spectrometers (XEDS) for chemical analysis which has proved very effective in meeting the needs of the research community. One of the TEM's is for high resolution each and the other as configured for its analytical capabilities. A Gatan parallel EELS system and XEDS system have been installed on the analytical microscope.

Future plans include image computing facilities, updated specimen preparation and photographic equipment, and specimen holders at high temperatures. This past year a large part of the use of these machines was devoted to characterization of high Tc materials and other ceramic materials.

Mechanical Properties

This laboratory is equipped with a modern universal mechanical testing machine, a spark cutting machine for preparing samples for analysis and a creep testing machine.

Experimental Materials Science Facility

This laboratory designed to provide 5,200 ft² of critically needed space consisting of eight laboratories was completed in 1989. Of the eight laboratories in this building, CMS personal occupy four, ERDC researchers use three, and one is used by INC-4. There are two labs for work on amorphous materials, one for chemical synthesis and characterization for sensor materials, two to support Scanning Tunnelling Microscopy (STM) activity, one for Thallium oxides, one for property measurements, and one for materials preparation.

Major modification for completing the Thallium lab was performed this year. All of the labs are now fully operational. The majority of the research carried out this last year in this lab has been on high Tc materials.

X-Ray Machine Laboratory

The 1600 ft² building was completed September 31, 1989, south of the Experimental Materials Laboratory. It is designed to house five x-ray machines and act as a central facility for these activities. Researchers from CMS, ERDC, P-10, and MST Division will use these machines. In the past, these machines had been spread out over several sites. The primary use of these machines will be for materials characterization. We now have five x-ray machines operating in this building, and it is fully operational.

Materials Science Laboratory

The new Materials Science Laboratory (MSL) that will house researchers from many Los Alamos organizations including CMS, MST, P, M, INC, CLS, T, and MEE is under construction as of April 1991. The Materials Science Laboratory (MSL) will be a modern facility built and equipped to safely conduct synthesis, processing, and characterization of new and novel materials to support programs of national interest in defense, energy, and the basic sciences.

The MSL building contains 27 laboratories, 15 support rooms, 49 offices which will house 59 people, a library, and a 72 seat sloping-floor lecture room in a 55,360 sq. ft., two-story, "H" shaped building. The building, access roads, parking lots, and landscaped areas will cover approximately 7 acres of a previously disturbed site. Facility construction began July 1991 and continue through 1992. Research apparatus procurement and installation will require at least one more year. The total project cost is \$29.3 million of which the building construction contract is approximately \$1 3M, the remainder is for research apparatus, additional building hardware, design, and management. Funding is provided by the Department of Energy's Defense Programs Weapons Activity.

Advances in today's high-technology programs depend upon the creation of materials that must satisfy very specific requirements which stretch the limits of materials capabilities, or require unusual combinations of properties. The ability to create materials-by-design requires an understanding of how to put atoms together to make a material and how to form it into the shapes required. This understanding is acquired through the interaction of scientists specializing in the synthesis of new materials and those who characterize the behavior of materials. The MSL will provide the necessary interactive environment and modern equipment; permitting novel material synthesis and detailed materials characterization. Knowledge gained through the study of materials under extreme conditions of temperature, pressure, strain, and strain rate is essential for the advancement of technology in commerce and weaponry.

Fundamental materials research performed in universities and materials processing developments occurring in industry are important elements that must be incorporated into our materials research and development. Los Alamos scientists must be able to effectively interact with these communities so that we can acquire the latest developments, thereby strengthening our ability to solve materials related technical problems. The MSL is located in an open (security clearances are not required) area adjacent to facilities housing most of the materials scientists at Los Alamos. The MSL provides facilities for un-cleared visitors to work in collaboration with Los Alamos staff and is designed to enhance communication among the occupants and those of the adjacent facilities.

The MSL will be equipped with state-of-the-art research equipment. The mating of computers with synthesis, processing, and characterization apparatus has revolutionized the world of materials science. Processes and tests are now better controlled, data more accurately acquired and presented, and manpower reduced for the creation of materials and the acquisition of information about their behavior. The limits of testing capability have been extended. The provision of this research equipment in the MSL will allow Los Alamos to remain competitive among the world's materials centers and allow us to apply this knowledge to the various programs of interest to the Laboratory and the Nation.

Scanning Tunnelling Microscopy (STM)/Atom Force Microscopy (AFM) Laboratory

The use of STM/AFM techniques for research at Los Alamos is in its infancy. Its importance is expected to grow and a central, outside the fence facility, available to Laboratory staff would play an important role in this development. A central facility could be operated by staff doing forefront research with STM/AFM. These researchers could provide training and support for divisions and programs utilizing STM/AFM.

Based upon the above considerations it decided to set-up an STM/AFM Laboratory in CMS for CM directorate wide activities. CMS has designated two labs for STM/AFM work. In collaboration with INC Division one STM/AFM machine will be installed early next fiscal year. From a collaborative effort with CLS Division a plan has emerged to install a STM/AFM machine with Ultra-High Vacuum capability. With this facility the Laboratory greatly expands its capability to study the surface structure and morphology of materials.

**X. RESEARCH PUBLICATIONS
AND
PRESENTATIONS**

PUBLICATIONS

1. "The Shape, Configuration and Stress Field of Twins and Martensite Plates"
T. E. Mitchell and J. P. Hirth
Acta Metallurgica Mater. 39, 1711-1717 (1991)
LA-UR-90-3422
2. "Importance of Structural Instability to High-Temperature Superconductivity"
A. Bussmann-Holder, Albert Migliori, Zachary Fisk, John L. Sarrao, and
S.-W. Cheong
Physical Review Letters
LA-UR-90-3445
3. "Ion Beam Materials Lab's Report to S.N.E.A.P. '90 (Symposium North East All
Personnel)"
Caleb R. Evans, Mark G. Hollander, and Joseph R. Tesmer
Report to be presented at S.N.E.A.P., October 22-25, 1990, Manhattan, KA
LA-UR-90-3517
4. "On Modeling Anisotropy in Deformation Processes Involving Textured Polycrystals with
Distorted Grain Shape"
Kapil K. Mathur, Paul R. Dawson, and U. F. Kocks
Mechanics of Materials
LA-UR-90-3525
5. "Nonlinearly Coupled Vibrational Modes and Self-Trapped States: Quantum Langevin
Theory and the Single Vibron Oscillator Case"
A. M. Clogston and H. Keith McDowell
Physical Review B 44, September 1, 1991
LA-UR-91-3650
6. "Theoretical Studies of the Alpha - Alpha' Transition in Cerium"
J. M. Wills, Olle Eriksson, and A. M. Boring
Physical Review Letters (paper)
LA-UR-90-3674
7. "Magnetic Properties of $R_2\text{CuO}_4$ Materials (R: Rare Earth)"
Zachary Fisk, Joe D. Thompson, S.-Wook Cheong, C. ReHori, S. B. Oseroff,
D. C. Vier, S. Schultz, M. Tovar, and R. Zysler
Studies of High Temperature Superconductors, ed. A. V. Narliker (book)
LA-UR-90-3723
8. "Nucleation and Growth of a BCC Fe Phase Deposited on a Single Crystal (001) Cu
Film"
J. Koike
Scripta Metallurgica
LA-UR-90-3786

9. "Re-Examination of the Kondo Resonance: Inconsistencies with the Gunnarson-Schonhammer Model"
A. J. Arko, R. S. List, R. J. Bartlett, P. Canfield, Z. Fisk, J. L. Smith,
J. Lawrence, J. Tang, D. Dessau, and B. Wells
NSLS 1991 Annual Report
LA-UR-90-3987
10. "Heavy-Mass State in Antiferromagnetic CeX_2Sn_2 Compounds"
Joe. D. Thompson, Ward P. Beyermann, Michael F. Hundley, Paul C. Canfield,
Zachary Fisk, James L. Smith, C. Godart, and M. Selsane
APS 1991 March Meeting
LA-UR-90-3988
11. "Specific Heat Measurements on Boron Substituted UBe_{13} "
Ward P. Beyermann, Robert H. Heffner, Michael F. Hundley, Joe D. Thompson,
James L. Smith, Zachary Fisk, and H. R. Ott
APS 1991 March Meeting, Cincinnati, OH, March 18-22, 1991
LA-UR-90-3989
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15. "Boson Mediated Model for High Temperature Superconductivity From Nambu-Eliasberg
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111. "Correlation Between Axial-Oxygen Anharmonicity and T_c in $\text{YBa}_2\text{Cu}_3\text{O}_7$ and Related Compounds"
J. Mustre de Leon, S. D. Conradson, I. Batistic, and A. R. Bishop
Phys. Rev. B, 44, 2422 (1991), Rapid Communication

112. "XAFS Analysis in the Anharmonic Limit; Application to Hi-T_c Superconductors and Ferrosilicates"
J. Mustre de Leon, S. D. Conradson, A. R. Bishop, I. D. Raistrick, I. Batistic, and W. E. Jackson
in X-ray Absorption Fine Structure VI, edited by S. Hasnain, (Ellis Horwood Ltd., Chichester, UK 1991).
113. "Characterization of a Split Axial-Oxygen Site in TlBa₂Ca₃Cu₄O₁₁ by EXAFS"
P. G. Allen, J. Mustre de Leon, S. D. Conradson, and A. R. Bishop
Phys. Rev. B (to appear November 1, 1991)
114. "Axial Centered Lattice Instabilities in Axial Oxygen in YBa₂Cu₃O₇: An Application of the Analysis of EXAFS in Anharmonic Systems"
Phys.. Rev. B (to appear December 1, 1991)
115. "A Polaron Origin for Anharmonicity of the Axial Oxygen in YBa₂Cu₃O₇"
J. Mustre de Leon, I. Batistic, A. R. Bishop, S. Trugman, and S. D. Conradson
Physical Review Letters, October 1991

112. "XAFS Analysis in the Anharmonic Limit; Application to Hi- T_c Superconductors and Ferrosilicates"
J. Mustre de Leon, S. D. Conradson, A. R. Bishop, I. D. Raistrick, I. Batistic, and W. E. Jackson
in X-ray Absorption Fine Structure VI, edited by S. Hasnain, (Ellis Horwood Ltd., Chichester, UK 1991).
113. "Characterization of a Split Axial-Oxygen Site in $TlBa_2Ca_3Cu_4O_{11}$ by EXAFS"
P. G. Allen, J. Mustre de Leon, S. D. Conradson, and A. R. Bishop
Phys. Rev. B (to appear November 1, 1991)
114. "Axial Centered Lattice Instabilities in Axial Oxygen in $YBa_2Cu_3O_7$: An Application of the Analysis of EXAFS in Anharmonic Systems"
Phys. Rev. B (to appear December 1, 1991)
115. "A Polaron Origin for Anharmonicity of the Axial Oxygen in $YBa_2Cu_3O_7$ "
J. Mustre de Leon, I. Batistic, A. R. Bishop, S. Trugman, and S. D. Conradson
Physical Review Letters, October 1991
116. "Interplanar Binding and Lattice Relaxation in a Graphite Di-Layer"
Samuel B. Trickey, F. Muller-Plathe, G. H. F. Dierchsen, and J. C. Boettger
Phys. Rev. B (accepted)
117. "Prediction of the Low-Pressure Phases in Lithium"
J. A. Nobel, Samuel B. Trickey, P. Blaha, K. Schwarz
Phys. Rev. B (accepted)

PRESENTATIONS

1. "Attempts to Solve Unwanted Charge Loss in NEC Team Tandem Accelerators"
J. R. Tesmer and C. J. Maggiore
Talk to be presented at the Small Tandem Workshop prior to the start of the 11th
Conference on the Applications of Accelerators in Research and Industry, U. of
North Texas, Denton, TX, November 4, 1990
LA-UR-90-3743
2. "De Haas-Van Alphen Effect in YBCO"
J. L. Smith, C. M. Fowler, B. L. Freeman, W. L. Hults, J. C. King, and
F. M. Mueller
March Meeting of the American Physical Society, March 18-22, 1991, Cincinnati,
OH
LA-UR-90-3781
3. "Large Low-Temperature Specific Heat in YbBiPt"
H. R. Ott, E. Felder, Ward P. Beyermann, Paul C. Canfield, Michael F. Hundley,
Zachary Fisk, and Joe D. Thompson
APS 1991 March Meeting, Cincinnati, OH, March 18-22, 1991
LA-UR-90-3993
4. "Pressure Studies of the Magnetic Phase Transition of the Heavy Fermion Compound
 $\text{Ce}(\text{Cu}_{1-x}\text{Ni}_x)_2\text{Ge}_2$ "
Guenter Sparn, Ward P. Beyermann, Paul C. Canfield, Zachary Fisk, and
Joe D. Thompson
APS 1991 March Meeting, Cincinnati, OH, March 18-22, 1991
LA-UR-90-3994
5. "Resonant Ultrasound of the Tetragonal-Orthorhombic Phase Transition in Sr Doped
 La_2CuO_4 "
Robert G. Leisure, John L. Sarrao, S.-W. Cheong, Paul C. Canfield,
Zachary Fisk, and Albert Migliori
APS 1991 March Meeting, Cincinnati, OH, March 18-22, 1991
LA-UR-90-3995
6. "Theoretical Studies of the Alpha - Alpha' Transition in Ce"
J. M. Wills, Olle Eriksson, and A. M. Boring
American Physical Society Meeting, Cincinnati, OH, March 12, 1991
LA-UR-90-4001
7. "Theoretical Studies of the Crystal Structures of the Light Actinides"
J. M. Wills, O. Eriksson, and A. M. Boring
American Physical Society Meeting, Cincinnati, OH, March 12, 1991
LA-UR-90-4002
8. "Observation of a Kondo-Like Feature at E_F in the Photoelectron Spectrum of Purely
Localized CeSb_2 "
Aloysious J. Arko, John J. Joyce, Roger J. Bartlett, Paul C. Canfield, and
Zachary Fisk
APS 1991 March Meeting, Cincinnati, OH, March 18-22, 1991
LA-UR-90-4049

9. "The Dzyaloshinskii-Moriya Interaction in the Cuprates"
D. Coffey, T. M. Rice, and F. C. Zhang
APS 1991 March Meeting, Cincinnati, OH, March 18-22, 1991
LA-UR-90-4097

10. "Nuclear Quadrupole Relaxation and Oxygen Diffusion in Almost-Stoichiometric $\text{La}_2\text{CuO}_{4.5}$ "
J. P. Vithayathil, Douglas E. MacLaughlin, P. C. Hammel, Robert H. Heffner, Paul C. Canfield, Zachary Fisk, and Sang Wook Cheong
APS 1991 March Meeting, Cincinnati, OH, March 18-22, 1991
LA-UR-90-4130

11. "Absence of ^{139}La NQR Anomaly Below 150 K in $\text{La}_2\text{CuO}_{4+\Delta}$ "
Douglas E. MacLaughlin, J. P. Vithayathil, P. Chris Hammel, Robert H. Heffner, Paul C. Canfield, Zachary Fisk, and S.-W. Cheong
APS 1991 March Meeting, Cincinnati, OH, March 18-22, 1991
LA-UR-90-4131

12. "Application of Muon Spin Relaxation to Observe Vortex Dynamics in Superconducting"
Masahiko Inui
APS Journal (March Meeting Issue)
LA-UR-90-4152

13. "Inconsistencies with the Single-Impurity Anderson Model in the Photoelectron Spectrum of Heavy Fermion YbCu_2Si_2 "
John Lawrence, Aloysious J. Arko, John Joyce, Roger J. Bartlett, Paul C. Canfield, Zachary Fisk, and James L. Smith
APS 1991 March Meeting, Cincinnati, OH, March 18-22, 1991
LA-UR-90-4181

14. " ^{139}La NMR Study of Magnetic Field Dependent Behavior in Single Crystal $\text{La}_2\text{CuO}_{4.8}$ "
P. Chris Hammel, Douglas E. MacLaughlin, Eric T. Ahrens, Robert H. Heffner, Paul C. Canfield, Zachary Fisk, and Martin P. Maley
APS 1991 March Meeting, Cincinnati, OH, March 18-22, 1991
LA-UR-90-4182

15. "Counterintuitive Temperature Dependence of the 'Kondo Resonance' in CeBe_{13} "
Aloysious J. Arko, R. Scott List, John J. Joyce, Roger J. Bartlett, Paul C. Canfield, Zachary Fisk, James L. Smith, J. M. Lawrence, and J. Tang
APS 1991 March Meeting, Cincinnati, OH, March 18-22, 1991
LA-UR-90-4183

16. "Metastable Phase Equilibrium and Glass Forming Range in Coevaporated $\text{Ni}_{100-x}\text{Zr}_x$ Thin Films"
J. B. Rubin and R. B. Schwarz
March 1991 Meeting of the American Physical Society, Cincinnati, OH,
March 18-22, 1991
LA-UR-90-4244

17. "Kinetics of Solid-State Amorphization in Ni/Zr Thin-Film Multilayers"
R. B. Schwarz and J. B. Rubin
March 1991 Meeting of the American Physical Society, Cincinnati, OH,
March 18-22, 1991
LA-UR-90-4245

18. "Temperature Dependence in Nambu-Eliashberg Theory of Superconductivity for Large
Lambda: Application to Angle-Resolved Photoemission Data"
J. C. Swihart, G. B. Arnold, and F. M. Mueller
March 1991 Meeting of the American Physical Society, Cincinnati, OH,
March 18-22, 1991
LA-UR-90-4246

19. "Boson Mediated Model for High Temperature Superconductivity from Nambu-Eliashberg
Inversion of Angle-Resolved Photoemission Data: $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8.8}$ "
F. M. Mueller, G. B. Arnold, and J. C. Swihart
March 1991 Meeting of the American Physical Society, Cincinnati, OH,
March 18-22, 1991
LA-UR-90-4247

20. "Growth of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ Films on Metallic, Single Crystal Disilicide Substrate"
Li Luo, X. D. Wu, R. E. Muenchausen, S. R. Foltyn, R. C. Dye,
C. J. Maggiore, and L. J. Schowalter
American Physical Society Meeting, Cincinnati, OH, March 18-22, 1991
LA-UR-90-4248

21. "De Haas-Van Alphen Effect in YBCO"
J. L. Smith, C. M. Fowler, B. L. Freeman, W. L. Hults, J. C. King, and
F. M. Mueller
March Meeting of the American Physical Society, March 18-22, 1991, Cincinnati,
OH
LA-UR-90-4268

22. "Irradiation-Induced Phase Transformation of Diamond Films"
Jun-Ichi Koike and Don M. Parkin
Proposal of experiment to be conducted at Argonne National Laboratory,
HVEM-Tandem Facility
LA-UR-90-4289

23. "Preparation of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ Thin Films for Passive Microwave Device Applications"
R. E. Muenchausen, X. D. Wu, S. R. Foltyn, D. W. Cooke, R. Taber, L. Luo,
R. C. Dye, and N. S. Nogar
Washington Materials Forum, February 28 - March 1, 1991, Washington, DC
LA-UR-90-4302

24. "Interface Between $\text{YBa}_2\text{Cu}_3\text{O}_{7.8}$ and Ion-Damaged $\text{YBa}_2\text{Cu}_3\text{O}_{7.8}$ "
Xin Di Wu, L. Luo, R. C. Dye, S. R. Foltyn, R. E. Muenchausen, and N. S. Nogar
MRS 1991 Spring Meeting, April 29 - May 4, 1991, Anaheim, CA
LA-UR-90-4303

25. "Preparation and Properties of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ Thin Films on Silicon Substrates Using CoSi_2 Buffer Layer"
 Li Luo, X. D. Wu, R. E. Muenchausen, S. R. Folytn, R. C. Dye, C. J. Maggiore, J. R. Jimenez, and L. J. Schowalter
 Washington Materials Forum, Washington, DC, February 28 - March 1, 1991
 LA-UR-90-4320
26. "The Gold/High Temperature Superconductor Interface; Metallicity of the Near Surface Region and a Search for the Proximity Effect"
 D. S. Dessau, Z.-X. Shen, B. O. Wells, W. E. Spicer, R. Scott List, Aloysious J. Arko, Roger J. Bartlett, Z. Fisk, S-W. Cheong, C. G. Olson, D. B. Mitzi, C. B. Eom, A. Kapitulnik, T. H. Geballe, and J. E. Schirber
 American Vac. Soc. Conference, Toronto, Canada, October 1990
 LA-UR-90-4359
27. "Zircona Reinforced-Molybdenum Disilicide Matrix Composites"
 John J. Petrovic, Richard E. Honnell, Terence E. Mitchell, Robert K. Wade, and Kenneth J. McClellan
 15th Annual Conference on Composites and Advanced Ceramics, January 13-16, 1991, Cocoa Beach, FL
 LA-UR-90-4367
28. "Hardness and Toughness Properties of Hiped'ed Pure Si_3N_4 and $\text{Si}_3\text{N}_4\text{SiC}$ "
 O. Unal and T. E. Mitchell
 Symposium on Ceramic Matrix Composites, April 23 - May 2, 1991, Cincinnati, OH
 LA-UR-90-4379
29. "Nucleation and Growth of In-Situ Deposited $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ Thin Films"
 R. E. Muenchausen, X. D. Wu, S. R. Foltyn, L. Luo, M. Hawley, K. M. Hubbard, R. C. Dye, A. D. Rollett, T. G. Schofield, C. C. Chang, R. Ramesh, T. S. Ravi, D. M. Hwang, X. X. Xi, T. Venkatesan, H. R. Wenk, and F. Heidelbach
 MRS 1991 Spring Meeting, April 29 - May 4, 1991, Anaheim, CA
 LA-UR-90-4424
30. "Characteristic of YBCO Thin Films on Si with an Epitaxial CoSi_2 Buffer Layer"
 Li Luo, X. D. Wu, R. E. Muenchausen, S. R. Folytn, R. C. Dye, C. J. Maggiore, J. R. Jimenez, and L. J. Schowalter
 1991 MRS Spring Meeting, Anaheim, CA, April 29 - May 3, 1991
 LA-UR-90-4430
31. "Magnetic Penetration Depth and Flux-Dynamics in Single-Crystal $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8.8}$ "
 D. R. Harshman, R. N. Kleiman, M. Inui, G. P. Espinosa, D. B. Mitzi, A. Kapitulnik, T. Pfiz, and D. Ll. Williams
 American Physical Society Meeting, Cincinnati, OH, March 17-21, 1991
 LA-UR-90-4438
32. "Boson Mediated Model for High Temperature Superconductivity from Nambu-Eliasberg Inversion of Angle-Resolved Photoemission Data: $\text{Bi}_2\text{Sr}_2\text{CaCu}_3\text{O}_{8.8}$ "
 F. M. Mueller, G. B. Arnold, and J. C. Swihart
 Workshop on Electronic and Mechanisms for High Temperature Superconductivity, January 3-9, 1991, Miami, FL (Invited)
 LA-UR-91-2

33. "Review of Pulsed Excimer Laser Deposition of High T_c Thin Films and Buffer Layers at Los Alamos National Laboratory"
 R. E. Muenchausen, X. D. Wu, L. Luo, S. R. Foltyn, R. C. Dye, K. M. Hubbard, A. D. Rollett, and N. S. Nogar
 International Conference on Metallurgical and Thin Films ICMCTF-91,
 April 22-26, 1991, San Diego, CA
 LA-UR-91-33
34. "Beam-Target Interactions Relevant to the Production of Large-Area $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ Coatings by Pulsed Laser Deposition"
 S. R. Foltyn, R. E. Muenchausen, K. M. Hubbard, K. C. Ott, W. B. Hutchinson, E. Peterson, L. Luo, R. C. Dye, X. D. Wu, and N. S. Nogar
 International Conference on Metallurgical and Thin Films ICMCTF-91,
 April 22-26, 1991, San Diego, CA
 LA-UR-91-34
35. "Thermodynamics of Plastic Instabilities and Applications to Strain Localization in Textured Sheets"
 U. F. Kocks
 Invited lecture of European Colloquim on "Microscopic and Macroscopic Plastic Deformation Instabilities," Metz, France, July 8-10, 1991
 LA-UR-91-128
36. "Neutron Powder Diffraction Study of Magnetic Order in Alpha Manganese Metal"
 A. C. Lawson, Z. Fisk, and M. Aronson
 LANSCE Experiment Report, Los Alamos National Laboratory, 1990 Run Cycle
 LA-UR-91-268
37. "Strain Release by Dislocation and Twin Generation in $\text{Ga/AsGa}_{1-x}\text{In}_x\text{As}$ Strained Layer Superlattices Grown on (001), (111), and (211) Substrates"
 T. E. Mitchell and O. Unal
 Microscopy of Semiconducting Materials Conference, March 25-28, 1991, London, UK
 LA-UR-91-326
38. "Investigation of a Hamiltonian with Two Sources of Anisotropy: The Dzyaloshinskii-Moriya and Single-Site Interactions"
 Dermot Coffey
 5th Joint MMM-Inter Mag Conference, Pittsburgh, pA, June 18-21, 1991
 LA-UR-91-329
39. "Shapes, Configuration, Stresses and Energies of Twins and Twin Arrays"
 T. E. Mitchell
 Workshop on the "Dynamics of Microstructures," Los Alamos, NM,
 February 25-27, 1991
 LA-UR-91-452
40. "Materials at Extremes"
 Don M. Parkin
 Presentation to be at the 2021 A. D. ConForum, March 14-15, 1991, Pheonix, AZ
 LA-UR-91-458

41. "Fermi Surface of YBCO by DVHA"
James L. Smith, C. Maxwell Fowler, Bruce L. Freeman, W. Larry Hults,
James C. King, and F. M. Mueller
Electronic Surface and Mechanisms for High Temperature Superconductivity,
January 3-9, 1991, Coral Gables, FL
LA-UR-91-459
42. "Bosonic Mechanism for High-Temperature"
F. M. Mueller, G. B. Arnold, and J. C. Swihart
The University of Miami on: Electronic Structure and Mechanisms for High
Temperature Superconductivity, January 3-9, 1991, Miami, FL
LA-UR-91-567
43. "Gap-Like Magnetic Excitations in the Neutron Scattering Response of Cerium₃ Bismuth₄
Platinum₃"
Andrea Severing, Joe D. Thompson, Paul C. Canfield, Zachary Fisk, and
Peter Riseborough
19th Rare Earth Research Conference, Lexington, KY, July 14-19, 1991
LA-UR-91-713
44. "Doping and Pressure Study of Uranium₃ Antimony₄ Platinum₃"
Paul C. Canfield, Michael F. Hundley, Alex Lacerda, Ward P. Beyermann,
Gunter Sparn, Joe D. Thompson, and Zachary Fisk
19th Rare Earth Research Conference, Lexington, KY, July 14-19, 1991
LA-UR-91-714
45. "Possible Heavy Fermion Behavior in New Rare Earth-Platinum-Gallium Compounds"
Paul C. Canfield, Joe D. Thompson, Ward P. Beyermann, Zachary Fisk,
Carol Burns, David Brunhart, Michael F. Hundley, Alex Lacerda, and Gunter Sparn
19th Rare Earth Research Conference, Lexington, KY, July 14-19, 1991
LA-UR-91-744
46. "Formation of Martensite in Nickel-Titanium Alloys by Negative Pressure Pulses"
R. B. Schwarz
"Dynamics of Microstructures" Workshop, Los Alamos, NM, February 25-27, 1991
LA-UR-91-745
47. "Dislocations and Plastic Deformation in MoSi₂"
T. E. Mitchell
High Temperature Structural Silicides Workshop, Gaithersburg, MD,
November 4-6, 1991
LA-UR-91-797
48. "Microstructure of Epitaxial YBa₂Cu₃O₇ Thin Films"
T. E. Mitchell
"Ceramic Superconductors" by the American Ceramic Society International Congress
on Ceramic Science and Technology, Orlando, FL, November 12-15, 1990
LA-UR-91-887

49. "Thermodynamics of Plastic Instabilities and Applications to Strain Localization in Textured Sheets"
U. F. Kocks
Workshop on "Microscopic and Macroscopic Deformation Instabilities," Universite Metz, France, July 8-11, 1991
LA-UR-91-888
50. "Synthesis and Properties of MoSi_2 Prepared by Mechanical Alloying"
R. B. Schwarz, S. Srinivasan, and J. J. Petrovic
First Workshop on "High Temperature Structural Silicides," NIST, Gaithersburg, MD, November 4-6, 1991 (Invited)
LA-UR-91-919
51. "Fermi Surface of YBCO by DHVA"
James L. Smith, C. Maxwell Fowler, Bruce L. Freeman, W. Larry Hults, James C. King, and Fred M. Mueller
The University of Miami Workshop on: Electronic Structure and Mechanisms for High Temperature Superconductivity, January 3-9, 1991, Miami, FL
LA-UR-91-964
52. "High Pressure Transport Properties of Alpha-Manganese"
M. C. Aronson, Zachary Fisk, Andrew C. Lawson, and Joe D. Thompson
International Conference on Magnetism, Edingburgh, Great Britian, September 2-6, 1991
LA-UR-91-995
53. "The Derivation of Effect Spin Hamiltonians and the Origin of the Magnetic Field Induced Transition in Orthorhombic La_2CuO_4 "
Dermot Coffey
Physical Phenomena at High Magnetic Fields, May 15-18, 1991, Tallahassee, FL
LA-UR-91-1015
54. "Strain Release in $\text{GaAs}/\text{Ga}_{1-x}\text{In}_x\text{As}$ Strained Superlattices Grown on (112) Substrates"
T. E. Mitchell and O. Unal
Microscopy of Semi-conducting Materials, Oxford, England, March 25-28, 1991
LA-UR-91-1043
55. "Application of Muon Spin Relaxation Experiment to the Vortex Dynamics of High Temperature Supercodnuctors"
Masahiko Inui
International Conference on Materials and Mechanisms of Superconductivity, High Temperature Superconductors, Kanazawa, Japan, July 22-26, 1991. Conference on Physical Phenomena at High Magnetic Fields, Florida State University, Tallahassee, FL, May 15-18, 1991
LA-UR-91-1061
56. "Synthesis of Intermetallic Materials by Mechanical Alloying"
Sreeram Srinivasan
Phillip-McKenna Labs,m Kennametal Inc., Greensburg, PA, May 6, 1991
LA-UR-91-1231

57. "Investigation of a Hamiltonian with Two Sources of Anisotropy: The Dzyaloshinskii-Moriya and Single-Size Interactions"
Dermot Coffey
5th joint MMM-Inter Mag Conference, Pittsburgh, PA, June 18-21, 1991
LA-UR-91-1275
58. "Non-Contact Ultrasonic-Spectroscopy Measurement of Elastic Constants"
R. B. Schwarz
28th Annual Technical Meeting, Society of Engineering Science, University of Florida, Gainesville, FL, November 6-8, 1991 (Invited talk)
LA-UR-91-1283
59. "Modeling the Anisotropy of Plasticity"
A. D. Rollett, U. F. Kocks, and M. G. Stout
ASM Materials Congress, Cincinnati, OH, October 20-24, 1991
LA-UR-91-1325
60. "DHVA 1991: Opportunities Using High Fields"
F. M. Mueller
Workshop "Physical Phenomena at High Magnetic Fields," May 15-18, 1991, Tallahassee, FL (Invited)
LA-UR-91-1360
61. "Recent Advances in the Synthesis of Amorphous Alloys"
Ricardo B. Schwarz
Tokyo University of Agriculture and Technology, Tokyo, Japan, May 13, 1991
LA-UR-91-1376
62. "Synthesis of Metastable Trialuminides by Mechanical Alloying"
R. B. Schwarz, S. Srinivasan, and P. Desch
Tokyo University of Agriculture and Technology, Tokyo, Japan, May 13, 1991
(Invited talk)
LA-UR-91-1377
63. "Metastable Phase Equilibria in Co-Deposited $\text{Ni}_{1-x}\text{Zr}_x$ Thin Films"
J. B. Rubin and R. B. Schwarz
Materials Research Society Symposia Proceedings, Spring 1991, Anaheim, CA
LA-UR-91-1487
64. "Kinetics of Solid-State Reactions in Ni-Zr Thin Films"
R. B. Schwarz and J. B. Rubin
Materials Research Society Symposia Proceedings, Spring 1991, Anaheim, CA
LA-UR-91-1488
65. "Metastable Phases in Aluminum-Based Intermetallics by Mechanical Alloying"
R. B. Schwarz, S. Srinivasan, and P. Desch
DOE-OBES Meeting, May 29-30, 1991, SNL, Los Alamos, NM (Poster)
LA-UR-91-1489

66. "Synthesis of Metastable Aluminum-Based Intermetallics by Mechanical Alloying"
R. B. Schwarz, S. Srinivasan, and P. Desch
International Symposium on Mechanical Alloying, Kyoto, Japan, May 7-10, 1991.
Proceedings to be published in Materials Science Forum, Trans. Tech. Publications
LA-UR-91-1490
67. "Epitaxial of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ Thin Films on Si Using CeO_2 Buffer Layers"
Li Luo, X. D. Wu, R. C. Dye, R. E. Muenchausen, S. R. Folytn, C. J. Maggiore,
and T. Inoue
Superconductivity and Applications, Buffalo, NY, September 24-26, 1991
(Invited talk)
LA-UR-91-1520
68. "Heavy Fermions in High Magnetic Fields"
Zachary Fisk and Joe D. Thompson
International Conference on Physical Phenomena at High Magnetic Fields,
Tallahassee, FL, May 15-18, 1991
LA-UR-91-1540
69. "Possible Heavy Fermion Behavior and Field-Induced Transitions in New Rare Earth
Platinum Gallium Compounds"
Alex Lacerda, Paul C. Canfield, Michael F. Hundley, Ward P. Beyermann,
Gunter Sparn, Joe D. Thompson, Zachary Fisk, Carol Burns, and David Burnhart
19th Rare Earth Conference. Journal of the Less-Common Metals
LA-UR-91-1544
70. "The U. S. National High Magnetic Field Laboratory: Status and Future"
J. E. Crow, N. Sullivan, and D. Parkin
3rd International Symposium on Research in High Magnetic Fields,
August 28-30, 1991, Tallahassee, FL
LA-UR-91-1588
71. "High-Temperature Plasticity in Copper Polycrystals"
Shuh Rong Chen and U. F. Kocks
DOE-OBES Meeting, May 20-30, 1991, Los Alamos, NM
LA-UR-91-1596
72. "Formation of Single Crystal Metallic NiSi_2 Thin Film on Amorphous SiO_2/Si "
Li Luo, C. J. Maggiore, R. F. Pinizzotto, H. Yang, and F. Namavar
38th Annual AVS Symposium and Topical Conference, Seattle, WA,
November 11-15, 1991
LA-UR-91-1678
73. "The Derivation of Effective Spin Hamiltonians and the Origin of the Magnetic Field
Induced Transition in Orthorhombic La_2CuO_4 "
Dermot Coffey
Physical Phenomena at High Magnetic Fields, Tallahassee, FL, May 15-18, 1991
LA-UR-91-1680
74. "Application of Muon Spin Relaxation Experiment to the Mixed State Superconductors"
Masahiko Inui and D. R. Harshmann
Physical Phenomena at High Magnetic Field, Tallahassee, FL, May 15-18, 1991
LA-UR-91-1685

75. "Research at Los Alamos Ion Beam Materials Laboratory"
 Carl J. Maggiore
 Encuentro Nacional Sobre Aceleradores, May 22-24, 1991, Mexico City, Mexico
 LA-UR-91-1731

76. "Texture Development in Cu-W Composites"
 W. J. Poole, U. F. Kocks, R. E. Bolmaro, and J. D. Embury
 12th Riso International Symposium "Metal Matrix Composites: Processing, Microstructure and Properties," Riso, Denmark, September 2-6, 1991
 LA-UR-91-1733

77. "Epitaxial Growth of Silicon on $\text{CoSi}_2(001)/\text{Si}(001)$ "
 Q. F. Xiao, J. R. Jimenez, L. J. Schowalter, L. Luo, T. E. Mitchell, and W. M. Gibson
 Materials Research Society, Anaheim, CA, April 29 - May 3, 1991
 LA-UR-91-1734

78. "dHvA Effect and Fermi Surface of YBCO"
 Clarence M. Fowler, Bruce L. Freeman, William L. Hults, James C. King, Fred M. Mueller, and James L. Smith
 OBES Materials Sciences Information and Review Meeting, May 29-30, 1991, Center for Materials Science, Los Alamos, NM
 LA-UR-91-1756

79. "Tribological Properties of Structures Formed by Ion and Excimer Laser Irradiation"
 M. Nastasi, J.P. Hirvonen, and T. R. Jervis
 Invited paper presented at the American Vacuum Society workshop on Mechanical and Material Characterization of Thin Films, Lakewood, CO, August 22, 1991
 LA-UR-91-1793

80. "Neutron Irradiation Effects in Bulk and Thin Film $(\text{Gd}, \text{Y})_1\text{Ba}_2\text{Cu}_3\text{O}_{7-x}$ "
 K. E. Sickafus, K. M. Hubbard, M. M. Chadwick, S. G. Boeke, C. J. Salgado, C. D. Kise, F. W. Clinard, Jr., W. A. Coghlan, K. A. Martin, D. E. Peterson, J. O. Willis, Y. J. Coulter, S. R. Foltyn, R. C. Dye, R. E. Muenchausen, M. P. Maley, D. M. Parkin, W. B. Wilson, and G. T. Ramsey
 Joint Los Alamos and Sandia National Laboratories, Albuquerque Information and Review Meeting of the Materials Sciences Programs sponsored by the Department of Energy Office of Basic Energy Sciences, May 29-30, 1991, Los Alamos, NM
 LA-UR-91-1794

81. "Effects of the Creation of Lattice Defects by the Decomposition of $\text{Ba}(\text{2})\text{Cu}(\text{3})\text{O}(\text{5}+\text{x})$ in $\text{YBa}(\text{2})\text{Cu}(\text{3}+\text{y})\text{O}(\text{7}-\text{x})$ ($0.1 < \text{y} < 1.5$)"
 Nicholas V. Coppa, W. Larry Hults, J. Yates, Eric J. Peterson, T. E. Mitchell, Dean E. Peterson, and James L. Smith
 1991 Spring MRS Meeting, Anaheim, CA, April 29 - May 3, 1991
 LA-UR-91-1809

82. "De Haas-Van Alphen Measurements in Superconductors Below Be_2 "
 F. M. Mueller
 3rd International Symposium on Research in High Magnetic Fields, Amsterdam, The Netherlands, August 1991
 LA-UR-91-1833

91. "Hardening in AlN Induced by Point Defects"
H. Suematsu, T. E. Mitchell, T. Iseki, and T. Yano
Materials Research Society Fall Meeting (1991), Boston, MA, December 2-6, 1991
LA-91-2285
92. "Electron Irradiation Effects of Diamond"
J. Koike, T. E. Mitchell, and D. M. Parkin
Materials Research Society Fall Meeting (1991), Boston, MA, December 2-6, 1991
LA-UR-91-2286
93. "High-Temperature Plasticity in Copper Polycrystals"
Shuh-Rong Chen and U. F. Kocks
Metalworking Technology, Inc., Johnstown, PA
LA-UR-91-2411
94. "High-Temperature Plasticity in FCC Polycrystals"
Shuh-Rong Chen and U. F. Kocks
TMS Fall Meeting, Cincinnati, OH, October 20-24, 1991
LA-UR-91-2412
95. "Superconducting Properties of YBCO Films on Sapphire with Oxide Buffer Layers"
Xin Di Wu, Steve R. Foltyn, Li Luo, Ross E. Muenchausen, and D. Wayne Cooke
Materials Research Society Fall Meeting, December 2-6, 1991, Boston, MA
LA-UR-91-2442
96. "Defects and Microstructure in High Tc Superconductors"
T. E. Mitchell
The Minerals Metals & Materials Society (TMS), San Diego, CA, March 1-5, 1992
LA-UR-91-2500
97. "Synthesis of Metallic Alloys with Metastable Phases and Microstructures"
R. B. Schwarz
Office of Basic Energy Sciences 1991 Annual Award, Washington, DC
LA-UR-91-2504
98. "Mechanical Alloying in the Synthesis of Intermetallics"
R. B. Schwarz, S. Srinivasan, and P. B. Desch
ASM-Europe Conference on "Synthesis, Processing, and Modelling of Advanced Materials," Paris, France, September 11-13, 1991
LA-UR-91-2568
99. "Excimer Laser Surface Processing for Tribological Applications"
T. R. Jervis
Colloquium presented at the Colorado College Physics Department, Colorado Springs, CO, April 8, 1991
LA-UR-90-2569
100. "Constitutive Relations for Dynamic Recrystallization"
U. F. Kocks
The Minerals Metals & Materials Society Meeting, San Diego, CA March 1-5, 1991
LA-UR-91-2570

83. "ZrO₂ Reinforced-MoSi₂ Matrix Composites"
 John J. Petrovic, Arun K. Bhattacharya, Richard E. Honnell, and Terence E. Mitchell
 Guidance and Evaluation Board Meeting for the DOE/CE Advanced Industrial
 Materials Program, June 10-11, 1991, Albuquerque, NM
 LA-UR-91-1848
84. "Crack Growth Resistance (R-Curve) Effects in Ceramics"
 S. Srinivasan
 University of Pittsburgh, July 1, 1991, Pittsburgh, PA (Invited talk)
 LA-UR-91-2123
85. "Aluminides with Ultrafine Microstructures: Synthesis and Properties"
 R. B. Schwarz
 Pre-conference Workshop on Nanocrystalline Materials, Third Canadian Materials
 Science Conference, Kingston, Ontario, Canada, June 18, 1991
 LA-UR-91-2124
86. "Structure-Process-Property Relations in Excimer Laser Surface Processed Ti-6Al-4V
 Alloy"
 T. R. Jervis, T. G. Zocco, and J. H. Steele, Jr.
 Presented at the Materials Research Society Symposium on Surface Chemistry and
 Beam Solid Interactions, November 26-30, 1990, Boston, MA
 LAUR-90-2184
87. "Orientation Dependent Epitaxial Growth of CeO₂ Layers on Si Substrates"
 T. Inoue, T. Ohsuna, Y. Yamamoto, Y. Sakurai, L. Luo, X. D. Wu, and
 C. J. Maggiore
 Materials REsearch Society, Boston, MA, December 2-6, 1991
 LA-UR-91-2198
88. "Non-Existence of "Kondo REsonance" in Photoemission Spectra of Ce Heavy
 Fermions: Possible Failure of the Anderson Model?"
 A. J. Arko, J. J. Joyce, P. C. Canfield, Z. Fisk, R. J. Bartlett, J. Lawrence, and
 J. Tang
 19th Rare Earth Research Conf., Lexington, KY, July 14-19, 1991
 LA-UR-91-2015
89. "Irradiation-Induced Amorphization as a Result of the Elastic Instability"
 Jun-Ichi Koike
 MRS Fall Meeting, Symposium A: Phase Formation and Modification by Beam-
 Solid Interactions, Boston, MA, December 2-6, 1991
 LA-UR-91-2035
90. "Growth of α -Axis Oriented, High Quality YBa₂Cu₃O_{7-x} Thin Films on Si"
 L. Luo, X. D. Wu, J. Koike, R. C. Dye, R. E. Muenchausen, S. R. Foltyn,
 Y. Coulter, C. J. Maggiore, and T. Inoue
 Materials Research Society Fall Meeting (1991), Boston, MA, December 2-6, 1991
 LA-UR-91-2282

101. "Dependence of Buried CoSi_2 Resistivity on Ion Implantation and Annealing Conditions"
J. M. Manke, F. Namavar, N. M. Kalkhoran, L. Luo, and J. T. McGinn
1991 Fall Materials Research Society Meeting, December 2-6, 1991, Boston, MA
LA-UR-91-2588
102. "Synthesis of Intermetallic Materials by Mechanical Alloying"
Sreeram Srinivasan and Ricardo B. Schwarz
International Conf. on High-Temperature Aluminides & Intermetallics,
September 16-19, 1991, San Diego, CA
LA-UR-91-2657
103. "Free Energy Difference Between Undercooled Liquids and Crystals"
R. B. Schwarz and P. Nash
Symposium on "Thermodynamics and Phase Equilibria of Metastable Phases,"
Annual AIME Meeting, San Diego, CA, March 1992
LA-UR-91-2799
105. "Photoemission of Cerium and Ytterbium Heavy Fermions: Inconsistencies in the Kondo Model"
John Joyce, Al Arko, Jon Lawrence, Paul Canfield, Joe Thompson, Z. Fisk, and R. Bartlett
To be presented at the Synchrotron Radiation center Users Meeting,
October 14-15, 1991, Madison, WI
LA-UR-91-2929
106. "De-Haas Van Alphen Measurements in Type II Superconductors"
Fred M. Mueller
University of Maryland, College Park, MD, September 24-25, 1991 (Invited)
LA-UR-91-3006
107. "Synthesis of Intermetallic Materials by Mechanical Alloying"
Sreeram Srinivasan
Dept. of Metallurgical Engineering, New Mexico Institute of Technology, Socorro, NM
September 25, 1991 (Invited)
LA-UR-91-3007
108. "An Anisotropic Convection Model for the Upper Mantle"
Y. C. Chastel, P. R. Dawson, K. Bennett, and H. R. Wenk
American Geophysical Union Meeting, San Francisco, CA, December 19, 1991
LA-UR-91-3008
109. "Copper Chloride, Revisited"
N. V. Coppa, W. P. Beyermann, J. D. Thompson, F. M. Mueller, and J. L. Smith
Phenomenology and Applications of High Temperature Superconductors, The Los Alamos Symposium: 1991, August 22-24, 1991
LA-UR-91-3024
110. "Phase Transformations in Superconducting and Non-Superconducting Perovskites"
T. E. Mitchell
ICOMAT-92, Monterey, CA, July 20-24, 1992
LA-UR-91-3040

112. "Pressured Orientation Development in Experimentally Deformed D₂O Ice Determined by Neutron Diffraction"
K. Bennett, H. R. Wenk, S. H. Kirby, W. B. Durham, and A. C. Lawson
American Geophysical Union Meeting, San Francisco, CA, December 19, 1991
LA-UR-91-3041
113. "Synthesis of Al/Al₃Ti Two-Phase Alloys by Mechanical Alloying"
S. Srinivasan, S. R. Chen, and R. B. Schwarz
Intl. Conf. on High-Temperature Aluminides and Intermetallics, San Diego, CA,
September 16-19, 1991; Proceedings to be published in Mater. Sci. and Engng.
LA-UR-91-3051
114. "Elastic Constants and the Structural Phase Transition in La_{2-x}Sr_xCuO₄"
John L. Sarrao, Ming Lei, Andres Stekel, Thomas M. Bell, Robert G. Leisure,
Lu J. Sham, A. Bussmann-Holder, William M. Visscher, I. Tanaka, H. Kojima, and
Albert Migliori
28th Annual Technical Meeting of the Society of Engineering Science, Gainesville,
FL, November 6-8, 1991 (Invited)
LA-UR-91-3141
115. "Excimer Laser Surface Processing of Metals and Ceramics for Tribological Applications"
T. R. Jervis
Invited presentation at the University of Michigan-Army Research Office Workshop
on Surface Science and Technology, Ann Arbor, MI, November 7-9, 1990
LA-UR-90-3171
116. "Plume Dynamics and Target Modification Effects in the Excimer Laser Vaporization of YBa₂Cu₃O_{7-δ}"
Steve R. Foltyn, Ross E. Muenchausen, Rob C. Dye, Xin Di. Wu, E. J. Peterson,
K. M. Hubbard, and L. Luo
14th International Conference on Lasers and Applications (Lasers '91)
LA-UR-91-3177
117. "Surface Modification for Tribological Applications in Space"
M. Nastasi, J-P Hirvonen, T. R. Jervis, and K. M. Hubbard
Presented at Aeromat '91 Long Beach, CA, May 20-25, 1991
LA-UR-90-3749
118. "Structure and Properties of Carbon Implanted Silicon Carbide"
J-P. Hirvonen, M. Nastasi, T. R. Jervis, and T. G. Zocco
Presented at the Eighth International Conference on Ion and Plasma
Assisted Techniques, Brussels, Belgium, May 21-24, 1991
LA-UR-90-4291
119. "Tribological Properties of Structures Formed by Surface Modification Techniques"
M. Nastasi, T. R. Jervis, and J-P. Hirvonen
Presented at the workshop on the Dynamics of Microstructures sponsored by the
Center for Materials Science, Los Alamos, NM, February 25-27, 1991

APPENDIX A

SEMINARS

SEMINARS SPONSORED BY
THE CENTER FOR MATERIALS SCIENCE
October 1, 1990 through September 30, 1991

- Dr. T. Suzuki, Hiroshima University
"Recent Results in Magneto-Acoustic Spectroscopies"
October 5, 1990
- Arturo Dominguez-Rodriguez, Universidad Seville
"Dislocations and Plasticity in Zirconia"
October 10, 1990
- Robert P. Messner, MIT (Postdoc)
"Formation Kinetics of Reaction Bonded Silicon Carbide Based Materials"
October 11, 1990
- Professor Arthur Heuer, Case Western Reserve University
"Mechanical Properties and Microstructure of Biological Ceramics - A vist to the World of Mollusks"
October 12, 1990
- Toshio Mukai, Nippon Steel Corporation
"Nd-Fe-B Permanent Magnets Prepared from Melt-Spin Ribbons"
October 26, 1990
- Carl Altsetter, University of Illinois at Urbana/Champaign
"Hydrogen Embrittlement of Face-Centered Cubic Alloys"
October 26, 1990
- Bill Neillis, Lawrence Livermore Laboratory
"Materials at the Extreme of Pressure and Temperature"
November 2, 1990
- Lars Nordstrom, Uppsala University
"Electronic Structure of $\text{Nd}_2\text{Fe}_{14}\text{B}$ and Other Rare Earth-Iron Compounds"
November 7, 1990
- K. J. Song, Rutgers University
"Ultra Thin Metal Film Induced Faceting on W Surface"
November 15, 1990
- Patrice Turichi, Lawrence Livermore National Laboratory
"From Electronic Structure Calculation to Alloy Phase Stability"
January 17, 1990
- Ellen Stechel, Sandia National Laboratory
"Model for Low Energy Electronic States for High Tc Cuprates Probed by X-Ray Absorption"
January 31, 1991

- E. W. Ong, LANSCE
"Interaction of Mercury in TiS_2 "
February 21, 1991
- C. A. Stone, UCLA (Postdoc Interviewee)
"The Influence of Low-Energy Particle-Surface Interactions on the Initial Stages of Thin Film Formation"
March 5, 1991
- M. V. Nevitt, Clemson University
"Phonon Softening in the Zirconia Transformation"
March 6, 1991
- E. N. Sickafus, Ford Motor Company
"Miniature Sensors for Automotive Control Systems -- an R&D Challenge"
March 11, 1991
- G. Aeppli, AT&T Bell Labs
"Magnetic Fluctuations in $\text{La}_{2-x}(\text{Sr,BA})_x\text{CuO}_4$ "
March 12, 1991
- Professor Toruo Kishi, University of Tokyo
"Quantitative Evaluation of Microcracks by Inverse Analysis of Acoustic Emission Signals, and Fracture Toughness of Ceramic Matrix Composites"
March 19, 1991
- Dr. Kazumi Hirano, MITI Research Institute
"Quantitative Evaluation of Microcracks by Inverse Analysis of Acoustic Emission Signals, and Fracture Toughness of Ceramic Matrix Composites"
March 19, 1991
- Francois Rossi, Centre d'Etudes et Recherches sur les Materiaux
"Diamond-Like Carbon Layers Obtained by Ion Beam Assisted Deposition: A Monte Carlo Approach"
May 7, 1991
- Jeffrey Wadsworth, Lockheed Missiles and Space Company, Inc.
"Recent Advances in Structural Aerospace Materials with an Emphasis on Superplasticity"
May 8, 1991
- David Clarke, UC Santa Barbara
"Microstructural Design for High Current Carrying Capacity Polycrystalline Superconductors"
May 20, 1991
- John R. Conrad, University of Wisconsin-Madison
"Plasma Physics, Materials Science, and Industrial Field Test Results Aspects of Plasma Source Ion Implantation"
May 31, 1991

John deBardillo, Inco Alloys International, Inc.

"New Industrial Applications of Mechanical Alloying: High Temperature Aluminum Alloys and High-Tc Superconductors"

June 6, 1991

Paul M. Tedrow, Francis Bitter National Magnet Laboratory

"Tunneling in Rare-Earth-Doped Superconductors"

June 6, 1991

Uli Hillebrecht, University of Dusseldorf

"Magnetism in Cr Overlayer on Iron"

June 28, 1991

John A. Mydosh, Rijksuniversiteit of Leiden

"The Magnetism and Superconductivity of URi_2Si_2 "

July 1, 1991

Y. Austin Chang, University of Wisconsin-Madison

"Reactions and Stability at the Metal-Semiconductor Interfaces"

July 5, 1991

Heinz Mecking, Technical University Hamburg-Marburg

"Strength and Ductility of Fe_3Al and $TiAl$ "

August 14, 1991

Boris Shapiro, Israel Institute of Technology

"Conductance Fluctuations Near the Mobility Edge"

August 15, 1991

Haruyuki Inui, Kyoto University

"Plastic Deformation of $TiAl$ Intermetallic Compounds with Lamellar Structure"

September 20, 1991

Shuji Hanada, Tokoku University

"Mechanical Properties of Intermetallic Compounds"

September 20, 1991

Osman Inal, New Mexico Tech

"Low-Voltage Plasma-Assisted Processing"

September 30, 1991

CONDENSED MATTER AND MATERIALS COLLOQUIUMS
SPONSORED BY
THE CENTER FOR MATERIALS SCIENCE
October 1, 1990 through September 30, 1991

- Stewart M. Lindsay, Arizona State University
"STM as a Probe of Electronic Structure of Adsorbates"
October 18, 1990
- Professor James Galligan, University of Connecticut
"Photoplasticity in 2-6 Compounds"
October 25, 1990
- Dermot Coffey, CMS
"Metamagnetism Behavior of CuO Planes"
November 8, 1990
- A. V. Balansky, University of Illinois/Landau Institute
"New Physics in Singlet Quantum Hall Effect-Spin 1/2 Anyons"
November 15, 1990
- Norman J. Wagner, T-12
"The Rheology of Polydisperse, Charged Colloids from Light Scattering and Small Angle Neutron Scattering: Comparison of Experimental Results and Theory"
November 29, 1990
- Mark Bourke, Imperial College/LANSCE
"Measurement of Residual Stress in Engineering Components by Neutron Diffraction"
December 6, 1990
- Mark Jarrel, University of Cincinnati
"Gap States in Dilute Magnetic Alloy Superconductors"
December 13, 1990
- A. K. Zurke, MST-5
"The Influence of Shock Pre-Strain and Peak Pressure on Spall Behavior of 4340 Steel"
December 20, 1990
- David A. Woodford, Rensselaer Polytech Institute
"Critical Properties Evaluation in High Temperature Composites"
January 10, 1991
- M. Fitzsimmons, Universitat Munchen/LANSCE
"X-Ray Reflectivity Measurements of (001) Au Surfaces and Twist Grain Boundaries"
January 17, 1991
- Sue N. Coppersmith, AT&T Bell Labs
"Defects in Random Elastic Media"
January 24, 1991
- S. E. Jones, The University of Alabama
"High Strain Rate Characterization of Materials Using the Taylor Impact Test"
February 14, 1991

I. E. Dzyaloshinski, UC Santa Barbara

"Time and Space-Parity Violation in Anyonic Conductors and Antiferromagnets"

February 28, 1991

Professor Takeshi Egami, University of Pennsylvania

"Local Structural Anomalies at Tc in HighTc Superconductors Observed by Neutron Scattering"

March 7, 1991

Lee Magness, U. S. Army Ballistic Research Lab

"Dynamic Deformation of Ballistic Materials"

March 14, 1991

Dr. Ronald W. Smith, Drexel University

"Mo/MoSi₂ Composites and Other MMC's Produced by Reactive Plasma Spray Forming"

March 21, 1991

Professor Susanne Raynor, Rutgers University

"A Hartree-Fock Approach to Highly Periodic Charged Systems"

March 28, 1991

Horst Meyer, Duke University

"The Shear Viscosity of ³He-⁴He Mixtures New Phase Transitions"

April 11, 1991

Gilles Montambaux, University of Paris

"Persistent Currents and Orbital Magnetism of Mesoscopic Systems"

April 18, 1991

Dr. Andrew J. Ouderkirk, 3M Center

"UV Laser Surface Modification of Semicrystalline Polymers"

April 25, 1991

Bernard R. Cooper, West Virginia University

"Predicting the Onset of Heavy Fermion Behavior"

May 22, 1991

Dr. Hironobu Ikeda, National Laboratory for High Energy Physics

"Spin Dynamic in the Percolation System"

May 30, 1991

John deBarbadillo, Inco Alloys International, Inc.

"New Industrial Applications of Mechanical Alloying: High Temperature Aluminum Alloys and High-Tc Superconductors"

June 6, 1991

David Schmeltzer, City university of New York

"Strongly Correlated Electrons: Application to Infinite U Hubbard Model"

June 20, 1991

Elizabeth A. Cooper, Northwestern University
 "Examination of the Reaction Kinetics of Oxide Superconductors Utilizing Impedance Spectroscopy and XRD"
 July 11, 1991

Dan Eliezer, University of Idaho
 "Hydrogen Effects in Titanium Aluminides"
 July 25, 1991

Cyrano DeDominicis, UCLA
 "Status of the Short-Ranged Microscopic Theory of Spin-Glass"
 August 1, 1991

John Ruvalds, University of Virginia
 "Fermi Surface Nesting in High Temperature Superconductors"
 August 15, 1991

Valery E. Frandkov, Rensselaer Polytechnic Institute
 "Main Regularities of 2-D Grain Growth"
 September 12, 1991

James E. Wittig, Vanderbilt University
 "Microstructural Characterization of Rapidly Solidified Metals"
 September 26, 1991

APPENDIX B

VISITORS

Robert G. Leisure
Colorado State University
Oct. 1, 1990-May 1, 1991
A. M. Boring, CMS
Collaborator

Altaf Carim
Penn State Univ.
October 1-2, 1990
Aug. 1-2, 1991
T. E. Mitchell, CMS
Official Visitor

Jacques Castaing
CNRS
October 10-11, 1990
T. E. Mitchell, CMS
Official Visitor

David Schmeltzer
City College, City Univ. of NY
October 18-24, 1990
June 16-29, 1991
Kevin Bedell, T-11
Consultant

James Galligan
Univ. of Connecticut
October 25-26, 1990
Ricardo Schwarz, CMS
Official Visitor

H. Sakamoto
Nippon Steel
October 26, 1990
T. E. Mitchell, CMS
Official Visitor

Toshio Mukai
Nippon Steel
October 26, 1990
T. E. Mitchell, CMS
Official Visitor

L.U.J. Thomas-Ogbuji
NASA Lewis Research Center
Nov. 19-20, 1990
T. E. Mitchell, CMS
Official Visitor

Valeri Vinokour
Academy of Sciences, USSR
Nov. 26-Dec. 4, 1990
August 22-24, 1991
L. J. Campbell, T-11
Kevin S. Bedell, T-11
Official Visitor

Cheng K. Saw
Hoechst-Celanese Corp.
Nov. 26-30, 1990
Ricardo Schwarz, CMS
Collaborator

Jorge Tirira
Lab. Pierre Sue
Nov. 12-13, 1990
Carl Maggiore, CMS
Official Visitor

Grylaine Ducouret
CNRS
Nov. 12-13, 1990
Carl Maggiore, CMS
Official Visitor

Gilbert Blondiaux
CNRS
Nov. 12-13, 1990
Carl Maggiore, CMS
Collaborator

Jean Luc Debrun
CNRS
Nov. 12-13, 1990
April 29-30, 1991
Aug. 8-10, 1991
Carl Maggiore, CMS
Collaborator

Roger Doherty
Drexel University
October 25-26, 1990
February 20-22, 1991
August 5-8, 1991
Tony Rollett, MST-6
U. F. Kocks, CMS
Collaborator

David Pines
University of Illinois/Urbana
Oct. 10-11 & 15, 1990
February 11-15, 1991
April 1, 1991
June 25-27, 1991
August 22-24, 1991
Sept. 4-6, 1991
Sept. 30, 1991
Don M. Parkin, CMS
Consultant

Gene Wells
 American Physical Society
 October 25-26, 1990
 A. M. Boring, CMS
 Official Visitor

Ker-Jar Song
 Rutgers University
 Nov. 14-16, 1990
 Shao-Ping Chen, T-11
 Official Visitor

Arthur Heuer
 Case Western Reserve Univ.
 October 12, 1990 (OV)
 Dec. 10-11, 1990
 Don M. Parkin, CMS
 Consultant

Thomas Tsakalakos
 Rutgers University
 October 27-30, 1990
 Chao-Ping Chen, T-11
 Official Visitor

Lars Nordstrom
 Univ. of Uppsala
 November 5-7, 1990
 Olle Eriksson, CMS
 Official Visitor

Dwight Adams
 Univ. of Florida
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

Guy Aubert
 Ecole Normale Supérieure
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

Greg Boebinger
 AT&T Bell Labs
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

James Brooks
 Boston University
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

Paul Chaikin
 Princeton University
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

J. Franse
 University of Amsterdam
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

Peter Gielisse
 Florida State University
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

Larry Jones
 Ames Laboratory
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

Michael Kaufman
 University of Florida
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

Mathias Leupold
 MIT
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

Alan T. Male
 Westinghouse Electric Corp.
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

James Ochsner
 DuPont
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

Jim Schirber
 Sandia National Lab
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

Hans J. Schneider-Muntau
 Max-Planck-Gesellschaft
 Nov. 5-6, 1990
 July 25-26, 1991
 Don M. Parkin, CMS
 Official Visitor

Gregory Stewart
 University of Florida
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

Carl Weggel
 MAGIC
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

Robert Weggel
 MIT
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

Peter Wyder
 Max-Planck-Gesellschaft
 Nov. 5-6, 1990
 Don M. Parkin, CMS
 Official Visitor

David Embury
 McMaster University
 Dec. 1-4, 1990
 August 5-8, 1991
 Don Parkin, CMS
 U. F. Kocks, CMS
 Collaborator

Tayfur Ozturk
 Middle East Technical Univ.
 October 9-24, 1990
 Fred Kocks, CMS
 Collaborator

Nuri Durlu
 New Mexico Tech.
 November 2, 1990
 A. D. Rollett, MST-6
 Official Visitor

Osman Inal
 New Mexico Tech.
 November 2, 1990
 Sept. 30, 1991
 A. D. Rollett, MST-6
 R. B. Schwarz, CMS
 Official Visitor

Alexander V. Balatsky
 University of Illinois
 Nov. 14-20, 1990
 Kevin Bedell, T-11
 Official Visitor

Wayne Worrell
 Univ. of Pennsylvania
 Dec. 10-11, 1990
 Don M. Parkin, CMS
 Consultant

John B. Wachtman
 Rutgers University
 Dec. 10-11, 1990
 Don M. Parkin, CMS
 Consultant

Gerd Rosenblatt
 UC Berkeley
 Dec. 10-11, 1990
 April 8-9, 1991
 Don M. Parkin, CMS
 Consultant

M. Brian Maple
 UC San Diego
 Dec. 10-11, 1990
 Don M. Parkin, CMS
 Consultant

James Mayer
 Cornell University
 Dec. 10-11, 1990
 Aug. 8-10, 1991
 Don M. Parkin, CMS
 Consultant

Khandker F. Quader
 Rutgers University
 Dec. 9-12, 1990
 Kevin S. Bedell, T-11
 Collaborator

Andrie Ruckenstein
Rutgers University
Dec. 10-14, 1990
Kevin Bedell, T-11
Collaborator

Jack Crow
Florida State University
Nov. 5-6, 1990
Don M. Parkin, CMS
Collaborator

Sebastian Doniach
Stanford University
Dec. 10-14, 1990
April 25-26, 1991
June 18-21, 1991
Aug. 12-24, 1991
Don M. Parkin, CMS
Consultant

Robert Schrieffer
UCSB
Dec. 10-12, 1990
February 4-5, 1991
June 24-28, 1991
August 19-30, 1991
Don M. Parkin, CMS
Kevin S. Bedell
Consultant

Peter Weinberger
Tech. Univ. of Vienna
Nov. 26-Dec. 1, 1990
July 8-27, 1991
A. M. Boring, CMS
Collaborator

Nelson E. Bickers
Univ. of Southern California
Dec. 11-15, 1990
Kevin Bedell, T-11
Official Visitor

Mark Jarrell
University of Cincinnati
Dec. 5-14, 1990
August 14-22, 1991
Kevin Bedell, T-11
Collaborator

Samuel B. Trickey
University of Florida
Jan. 2 - May 2, 1991
A. M. Boring, CMS
Collaborator

Peter Riseborough
Polytech University
Jan. 11-18, 1991
A. M. Boring, CMS
Collaborator

Paul Dawson
Cornell University
Jan. 14-18, 1991
June 3-7, 1991
August 5-8, 1991
Fred Kocks, CMS
Collaborator

Jon Lawrence
UC Irvine
Jan. 11-20, 1991
July 19-Aug. 31, 1991
Joe Thompson, P-10
Collaborator

Per Bak
Brookhaven National Lab.
Feb. 25-Mar. 1, 1991
Richard LeSar, T-11
Official Visitor

Paul Meakin
E.I. duPont de Nemours & Co.
Feb. 25-Mar. 1, 1991
Alan Bishop, T-11
Official Visitor

Michael Ashby
Univ. of Cambridge
Jan. 11-13, 1991
August 4-16, 1991
Fred Kocks, CMS
Consultant

Rudy Wenk
UC Berkeley
Jan. 7-11, 1991
May 15-Sept. 30, 1991
Fred Kocks, CMS
Collaborator

Per Soderlind
University of Uppsala
Dec. 1-19, 1990
A. M. Boring, CMS
Guest Scientist

Hartmut Monien
University of Illinois
Dec. 11-21, 1990
August 12-24, 1991
Kevin Bedell, T-11
Collaborator

Sue N. Coppersmith
AT&T Bell Labs
Jan. 23-25, 1991
Stuart Trugman, T-11
Collaborator

William Moshier
Martin-Marietta
Jan. 22-25, 1991
T. E. Mitchell, CMS
Visitor

David A. Woodford
Rensselaer Polytechnic Inst.
Jan. 10-11, 1991
A. D. Rollett, MST-6
Official Visitor

Patrice Truchi
Lawrence Livermore Nat. Lab
Jan. 17, 1991
Ricardo Schwarz, CMS
Visitor

Clare Yu
Univ. of California/Irvine
Jan. 19-Feb. 16, 1991
Sept. 20-24, 1991
Mike Boring, CMS
Collaborator

Ellen Stechel
Sandia Nat. Lab., Albuquerque
January 30-31, 1991
Kevin Bedell, T-11
Official Visitor

Ward Beyermann
January 15-Sept. 30, 1991
A. M. Boring, CMS
Collaborator

Tuan-Anh Tran
UC Santa Barbara
February 4-5, 1991
Kevin Bedell, T-11
Official Visitor

Mario Palumbo
Purdue University
February 4-15, 1991
Kevin Bedell, T-11
Official Visitor

Elihu Abrahams
Rutgers University
February 11-15, 1991
June 24-28, 1991
August 19-24, 1991
Sept. 23-27, 1991
Kevin Bedell, T-11
Consultant

Toni Schneider
IBM-Zurich
February 11-March 8, 1991
Kevin Bedell, T-11
Collaborator

Kim Christensen
Brookhaven Nat. Lab
Feb. 25-27, 1991
Richard LeSar, T-11
Visitor

Kenneth C. Ludema
University of Michigan
Feb. 25-27, 1991
Richard LeSar, T-11
Visitor

Ladislav P.J. Kubin
CNRS-ONERA
Feb. 21-27, 1991
Alan Bishop, T-11
Official Visitor

Robert F. Cook
Rice University
Feb. 25-27, 1991
A. D. Rollett, MST-6
Official Visitor

Michael Bocek
University of Karlsruhe
Feb. 24-Mar. 1, 1991
Alan Bishop, T-11
Official Visitor

Lee Tanner
LLNL
Feb. 25-27, 1991
Alan Bishop, T-11
Official Visitor

David Srolovitz
Univ. of Michigan
Feb. 25-27, 1991
Alan Bishop, T-11
Collaborator

Michael Kassner
Oregon State University
Feb. 25-27, 1991
A. D. Rollett, MST6
Official Visitor

Gerhard Barsch
Penn. State University
Feb. 25-27, 1991
Alan Bishop, T-11
Collaborator

J. W. Sethna
Cornell University
Feb. 25-27, 1991
Alan Bishop, T-11
Official Visitor

Lu Jeu Shan
UC San Diego
March 1 - August 31, 1991
A. M. Boring, CMS
Consultant

Carlos Tomé
Universidad Nacional de Rosario
March 16-24, 1991
Fred Kocks, CMS
Collaborator

Horst Meyer
Duke University
April 11-12, 1991
R. Ecke, P-10
Official Visitor

Gerhard Schadler
ETH Zurich
March 25-April 5, 1991
A. M. Boring, CMS
Collaborator

Gabriel Aepli
AT&T Bell Labs
March 11-13, 1991
August 22-24, 1991
R. Robinson, LANSCE
Kevin S. Bedell, T-11
Official Visitor

M. V. Nevitt
Clemson University
March 6, 1991
Fred Kocks, CMS
Official Visitor

Takeshi Egami
Univ. of Pennsylvania
March 6-7, 1991
Ricardo B. Schwarz, CMS
Official Visitor

Lee Magness
U.S. Army Ballistic Res. Lab
March 13-14, 1991
A. D. Rollett, MST-6
Official Visitor

Edward N. Sickafus
Ford Motor Company
March 11, 1991
Kurt Sickafus, MST-4
Official Visitor

Sven A. Rosengren
University of Uppsala
February 26-March 1, 1991
J. L. Smith, ERDC
Collaborator

Joe Stockel
CIA
February 14, 1991
Ricardo Schwarz, CMS
Official Visitor

Supramanian Srinivasan
Texas A&M Univ.
February 14, 1991
Ricardo Schwarz, CMS
Official Visitor

Arno Kampf
UC Santa Barbara
March 28-April 5, 1991
Kevin Bedell, T-11
Collaborator

Susanne Raynor
Rutgers University
March 26-28, 1991
F. Dowell, T-12
Collaborator

Kazumi Hirano
MITI Research Inst., Tokyo
March 19, 1991
Fred Kocks, CMS
Official Visitor

Toruo Kishi
University of Tokyo
March 19, 1991
Fred Kocks, CMS
Official Visitor

Gilles J. Montambaux
Univ. of Paris
April 18-19, 1991
Stuart Trugman, T-11
Official Visitor

Naresh Thadhani
New Mexico Tech.
April 4, 1991
June 3-7, 1991
Ricardo Schwarz, CMS
Collaborator

Francois Rossi
CEREM
May 3-8, 1991
Michael Nastasi, MST-7
Collaborator

David R. Clarke
Univ. of Calif. Santa Barbara
May 20-21, 1991
August 5-16, 1991
T. E. Mitchell, CMS
U. F. Kocks, CMS
Consultant

Paul M. Tedrow
MIT
June 5-6, 1991
Fred Mueller, CMS
Official Visitor

John deBarbadillo
Inco Alloys International, Inc.
June 6-7, 1991
Ricardo Schwarz, CMS
Official Visitor

Baird H. Brandow
June 12-Sept. 30, 1991
A. M. Boring, CMS
Guest Scientist

S. N. Basu
Boston University
July 1 - Aug. 2, 1991
T. E. Mitchell, CMS
Collaborator

Loic Mathieu
Ecole Central Paris
July 15 - Aug. 30, 1991
T. E. Mitchell, CMS
Student Guest Scientist

Stuart R. MacEwen
Alcan International Limited
May 29-30, 1991
August 5-8, 1991
Fred Kocks, CMS
Official Visitor

Uli Hillebrecht
University of Dusseldorf
June 27-28, 1991
A. M. Boring, CMS
Official Visitor

Boris Ivlev
L. D. Landau Inst.
July 22-Aug. 24, 1991
Kevin Bedell, T-11
Collaborator

Laszlo Mihaly
SUNY at Stony Brook
Aug. 22-24, 1991
Kevin Bedell, T-11
Official Visitor

Aharon Kapitulnik
Stanford University
August 22-24, 1991
Kevin Bedell, T-11
Official Visitor

Guy Deutcher
Tel-Aviv University
Aug. 22-24, 1991
Kevin Bedell, T-11
Official Visitor

Veli-Tapani Kuokkala
Tampere Inst. of Technology
August 5-23, 1991
R. B. Schwarz, CMS
Collaborator

Heinrich Mecking
Technical University
August 5-20, 1991
Fred Kocks, CMS
Collaborator

Pradeep Kumar
University of Florida
July 15-31, 1991
Fred Mueller, CMS
Collaborator

Douglas Scalapino
UCSB
Aug. 19-24, 1991
Don M. Parkin
Consultant

Abheya K. Datye
Univ. of New Mexico
July 15, 1991
T. E. Mitchell, CMS
Collaborator

Bryan R. Coles
Imperial College of Sci. & Tech.
August 1-23, 1991
J. L. Smith, ERDC
Collaborator

Philip Nash
Illinois Institute of Technology
June 17-July 26, 1991
Ricardo Schwarz, CMS
Collaborator

Hans Rudi Ott
ETH-Honggerberg, Zurich
Aug. 11-17, 1991
A. M. Boring, CMS
Collaborator

Maurice Rice
ETH-Honggerberg, Zurich
August 22-24, 1991
Don M. Parkin, CMS
Kevin S. Bedell, T-11
Consultant

Frans Spaepen
Harvard University
August 5-16, 1991
U. F. Kocks, CMS
Terry Mitchell, CMS
Consultant

David Meltzer
University of Florida
August 22-24, 1991
Kevin Bedell, T-11
Official Visitor

John P. Hirth
Washington State Univ.
August 5-16, 1991
U. F. Kocks, CMS
Consultant

A. Bussmann-Holder
Max-Planck-Institute
Aug. 20-25, 1991
A. Bishop, T-11
Official Visitor

Dan Eliezer
University of Idaho
July 25, 1991
Ricardo Schwarz, CMS
Official Visitor

John Ruvalds
University of Virginia
August 15-16, 1991
Fred M. Mueller, CMS
Official Visitor

John A. Mydosh
Rijksuniversiteit of Leiden
July 1-3, 1991
Kevin S. Bedell, T-11
Official Visitor

Y. Austin Chang
University of Wisconsin
July 5, 1991
Ricardo B. Schwarz, CMS
Official Visitor

R. Soderlind
Uppsala University
July 4-7, 1991
A. M. Boring, CMS
Official Visitor

V. Fradkov
Univ. of Pennsylvania
Sept. 12-13, 1991
A. D. Rollett, MST-6
Official Visitor

John W. Wilkins
Ohio State University
August 19-24, 1991
A. M. Boring, CMS
Collaborator

Boris Shapiro
Technion, Haifa
July 29-Aug. 26, 1991
Stuart Trugman, T-11
Collaborator

John Stringer
EPRI
August 21, 1991
Terry Mitchell, CMS
Official Visitor

Shuji Hanada
Tohoku University
Sept. 20, 1991
S-P. Chen, T-11
Official Visitor

A. Chiba
Tohoku University
Sept. 20, 1991
S-P. Chen, T-11
Official Visitor

Haruyuki Inui
Kyoto University
Sept. 20, 1991
T. E. Mitchell, CMS
Official Visitor

Vladimir Kogan
Ames Laboratory
Aug. 12-24, 1991
Larry Campbell, T-11
Collaborator

APPENDIX C

WORKSHOPS

NATIONAL HIGH MAGNETIC FIELD LABORATORY
Magnet Design Workshop
November 5-6, 1990
Center for Materials Science
Los Alamos, NM 87545

November 5, 1990

8:30 - 9:00 a.m.	Introduction - Don M. Parkin (LANL) - J. E. Crow (FSU)
9:00 - 10:15	DC Magnets and Discussion
10:15 - 10:30	Break
10:30 - 11:45	Long Pulsed Magnets and Discussion
11:45 - 1:00 p.m.	Lunch
1:00 - 1:30	20 MW DC Power Supply
1:30 - 2:00	CPRF 1430 MVA Generator
2:00 - 2:30	Power Supply Discussion
2:30 - 2:45	Break
2:45 - 3:30	High Strength, High Conductivity (thermal, electrical) Cu Alloys
3:30 - 4:15	Other Materials (Los Alamos)
4:15 - 5:00	Materials Discussion

November 6, 1990

8:30 - 9:45 a.m.	Capacitor Driven Magnets and Discussion
9:45 - 10:15	Instrumentation for Pulsed Magnets (Los Alamos)
10:15 - 10:30	Break
10:30 - 11:00	Instrumentation (continued)
11:00 - 12:00 p.m.	Summary Discussion
12:00 - 1:30	Lunch
1:30 - 4:00	Joint Discussion - establishment of working agreements

List of Attendees
Magnet Design Workshop
Center For Material Science (Seminar Room)
Los Alamos National Laboratory
November 5-6, 1990

Dwight Adams
Physics Department
215 Williamson Hall
University of Florida
Gainesville, FL 32611

Guy Aubert
Ministry of Education
Ecole Normale Supérieure
46, Alleg D-Italie
69369 Lyonfieder 07, France

Evan Ballard
Los Alamos National Laboratory
CTR-4
Mailstop E536
Los Alamos, NM 87545

Gloria Bennett
Los Alamos National Laboratory
CTR-4
Mailstop F644
Los Alamos, NM 87545

Greg Boebinger
AT&T Bell Laboratories
Rm. 1-D-208
600 Mountain Avenue
Murray Hill, NJ 07974

Heinrich Boenig
Los Alamos National Laboratory
CTR-4
Mailstop F644
Los Alamos, NM 87545

James S. Brooks
Boston University
Dept. of Physics
590 Commonwealth Ave.
Boston, MA 02215

Paul Chaikin
Princeton University
Dept. of Physics
Jadwin Hall, P.O. Box 708
Princeton, NJ 08544

Jack Crow
Dept. of Physics
Martech
Florida State University
Tallahassee, FL 32306

Max Fowler
Los Alamos National Laboratory
M-6
Mailstop J970
Los Alamos, NM 87545

J. Franse
University of Amsterdam
Physics Department
Valckenierstraat 65
1018XE Amsterdam, The Netherlands

Bruce Freeman
Los Alamos National Laboratory
M-6
Mailstop J970
Los Alamos, NM 87545

P. Gielisse
Dept. of Physics
Martech
Florida State University
Tallahassee, FL 32306

Jim Goforth
Los Alamos National Laboratory
M-6
Mailstop J970
Los Alamos, NM 87545

Mary Ann Hill
Los Alamos National Laboratory
MST-6
Mailstop G770
Los Alamos, NM 87545

Larry Jones
Ames Laboratory
114 Metals Dev. Building
Iowa State University
Ames, IA 50011-3020

Michael Kaufman
Materials Science and Engineering
132 Rhines Hall
University of Florida
Gainesville, FL 32611

Mathias Leupold
M.I.T.
Building NW 14-3220
150 Albany St.
Cambridge, MA 02139

E. A. Lopez
Los Alamos National Laboratory
CTR-4
Mailstop E536
Los Alamos, NM 87545

Alan T. Male
Manager, Adv. Proc. & Development
Science & Technology Center
Westinghouse Electric Corporation
Pittsburgh, PA 15235

Joe Minervini
Los Alamos National Laboratory
CTR-4
Mailstop F644
Los Alamos, NM 87545

Fred M. Mueller
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

James Ochsner
Dupont
Electronics Dept.
Wilmington, DE 19880

Henn Oona
Los Alamos National Laboratory
M-6
Mailstop J970
Los Alamos, NM 87545

Don M. Parkin
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Bob Reinovsky
Los Alamos National Laboratory
M-6
Mailstop J970
Los Alamos, NM 87545

Dwight Rickle
Los Alamos National Laboratory
M-6
Mailstop J970
Los Alamos, NM 87545

John Rogers
Los Alamos National Laboratory
CTR-4
Mailstop F644
Los Alamos, NM 87545

James Schirber
Sandia National Laboratory
P.O. Box 5800
1150, Bldg. 806
Albuquerque, NM 87185

Joe Schillig
Los Alamos National Laboratory
CTR-4
Mailstop F644
Los Alamos, NM 87545

Hans J. Schneider-Muntau
Max-Planck Institut fur Festkor.
Hochfeld-Magnetlabor
Grenoble
France

Jim Sims
Los Alamos National Laboratory
CTR-4
Mailstop F644
Los Alamos, NM 87545

Gregory Stewart
Physics Department
215 Williamson Hall
University of Florida
Gainesville, FL 32011-2085

Carl Storm
Los Alamos National Laboratory
M-DO
Mailstop P915
Los Alamos, NM 87545

Phil Thullen
Los Alamos National Laboratory
CTR-DO
Mailstop F640
Los Alamos, NM 87545

Carl Weggel
MAGIC
5945 Pacific Center Blvd.
Suite 510
San Diego, CA 92121

Robert J. Weggel
M.I.T.
Francis Bitter National Magnet Laboratory
Building 14-3220, 150 Albany St.
Cambridge, MA 02139

Peter Wyder
Hochfeld-Magnetlabor
25, Av.Des Martyrs - 166 X
F-38042 Grenoble Cedex
France

Center for Materials Science
External Advisory Committee Meeting
December 10-11, 1990

CMS Seminar Room

December 10, 1990

7:30	Breakfast at Otowi Cafeteria
8:30 - 10:20	CMS Issues - D. Parkin, M. Boring
10:20 - 10:30	1991 Summer Research Group
U. F. Kocks (CMS)
Scientific Program	
10:30 - 11:15	Toward Simpler Mechanisms for HTSC: Recent IANL Evidence
F. M. Mueller (CMS)
11:15 - 12:00	High Temperature Superconductors and Highly Correlated
Electron Materials
Z. Fisk (CMS)
12:00 - 1:30	Working Lunch - Parkin, Boring, EAC
1:30 - 2:00	Advanced Studies Program
R. J. Schrieffer, UC Santa Barbara (CMS)
2:00 - 2:30	f-electron systems
O. Eriksson (CMS)
2:30 - 3:00	Amorphization in NiTi
J. Koike (CMS)
3:00 - 3:30	Pulsed Laser Deposition of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ Thin Films
Ross Muenchausen (ERDC)
3:30 - 4:00	Microstructural Evolution during the Processing of
BSCCO/TBCCO - Silver Composite Conductors
Dave Phillips, MST-4
4:00 - 5:00	Tour of CPRF Generator
5:15 - 6:15	Reception - University House

December 11, 1990

New Directions

- 8:30 - 9:00 Proposed Accelerator Mass Spectroscopy at IBML
C. J. Maggiore (CMS)
- 9:00 - 9:30 Theory Institute
K. Bedell (T-11)
- 9:30 - 10:00 Tunable, Ultraviolet Laboratory Light Source
A. J. Arko (P-10)
- 10:00 - 12:15 EAC Caucus
- 12:15 - 1:30 E. Wewerka/R. Jensen

Adjourn

List of Attendees
 External Advisory Committee
 Center For Materials Science (Seminar Room)
 Los Alamos National Laboratory
 December 10-11, 1990

Al Arko
 Los Alamos National Laboratory
 P-10
 Mail Stop K764
 Los Alamos, NM 87545

Kevin Bedell
 Los Alamos National Laboratory
 T-11
 Mail Stop K765
 Los Alamos, NM 87545

Alan Bishop
 Los Alamos National Laboratory
 T-11
 Mail Stop B262
 Los Alamos, NM 87545

A. M. Boring
 Los Alamos National Laboratory
 CMS
 Mail Stop K765
 Los Alamos, NM 87545

Shuh-Rong Chen
 Los Alamos National Laboratory
 CMS
 Mail Stop K765
 Los Alamos, NM 87545

Dermot Coffey
 Los Alamos National Laboratory
 CMS
 Mail Stop K765
 Los Alamos, NM 87545

Olle Eriksson
 Los Alamos National Laboratory
 CMS
 Mail Stop K765
 Los Alamos, NM 87545

Doyle Evans
 Los Alamos National Laboratory
 ET-ACV
 Mail Stop F650
 Los Alamos, NM 87545

Zack Fisk
 Los Alamos National Laboratory
 CMS
 Mail Stop K765
 Los Alamos, NM 87545

Arthur Heuer
 Case Western Reserve University
 Materials Science and Engineering
 Cleveland, OH 44106

Mark Hollander
 Los Alamos National Laboratory
 CMS
 Mail Stop K765
 Los Alamos, NM 87545

Masahiko Inui
 Los Alamos National Laboratory
 CMS
 Mail Stop K765
 Los Alamos, NM 87545

Reed Jensen
 Los Alamos National Laboratory
 ADCM
 Mail Stop A102
 Los Alamos, NM 87545

U. Fred Kocks
 Los Alamos National Laboratory
 CMS
 Mail Stop K765
 Los Alamos, NM 87545

Jun Koike
 Los Alamos National Laboratory
 CMS
 Mail Stop K765
 Los Alamos, NM 87545

Li Luo
 Los Alamos National Laboratory
 CMS
 Mail Stop K765
 Los Alamos, NM 87545

Carl Maggiore
Los Alamos National Laboratory
CMS
Mail Stop K765
Los Alamos, NM 87545

M. Brian Maple
University of California at San Diego
Physics Department
La Jolla, CA 92093

James W. Mayer
Cornell University
Materials Science Department
Ithaca, NY 14853

Terry Mitchell
Los Alamos National Laboratory
CMS
Mail Stop K765
Los Alamos, NM 87545

Fred Mueller
Los Alamos National Laboratory
CMS
Mail Stop K765
Los Alamos, NM 87545

Don Nye
Los Alamos National Laboratory
CMS
Mail Stop K765
Los Alamos, NM 87545

Don Parkin
Los Alamos National Laboratory
CMS
Mail Stop K765
Los Alamos, NM 87545

Warren Poole
Los Alamos National Laboratory
CMS
Mail Stop K765
Los Alamos, NM 87545

Rod Quinn
Los Alamos National Laboratory
CMS
Mail Stop K765
Los Alamos, NM 87545

Tony Rollett
Los Alamos National Laboratory
MST-6
Mail Stop K765
Los Alamos, NM 87545

Jim Rubin
Los Alamos National Laboratory
CMS
Mail Stop K765
Los Alamos, NM 87545

Don Sandstrom
Los Alamos National Laboratory
MST-DO
Mail Stop G756
Los Alamos, NM 87545

Robert Schrieffer
Department of Physics
University of California, Santa Barbara
Santa Barbara, CA 93106

Ricardo Schwarz
Los Alamos National Laboratory
CMS
Mail Stop K765
Los Alamos, NM 87545

Jim F. Smith
Los Alamos National Laboratory
CMS
Mail Stop K765
Los Alamos, NM 87545

Sreeram Srinivasan
Los Alamos National Laboratory
CMS
Mail Stop K765
Los Alamos, NM 87545

Carl Storm
Los Alamos National Laboratory
M-DO
Mail Stop P915
Los Alamos, NM 87545

Joe Tesmer
Los Alamos National Laboratory
CMS
Mail Stop K765
Los Alamos, NM 87545

Ozer Unal
Los Alamos National Laboratory
CMS
Mail Stop K765
Los Alamos, NM 87545

Wesley Unruh
Los Alamos National Laboratory
ADAL
Mail Stop A134
Los Alamos, NM 87545

John B. Wachtman, Jr.
Rutgers University
Ceramics Research Center
Piscataway, NJ 08854

Wayne Worrell
University of Pennsylvania
119 Towne Building
Department of Materials Science
and Engineering
Philadelphia, PA 19104

Pascal Yvon
Los Alamos National Laboratory
CMS
Mail Stop K765
Los Alamos, NM 87545

Dynamics of Microstructures Workshop
 CMS Seminar Room
 Agenda
 February 25-27, 1991
 Center for Materials Science and Center For Nonlinear Studies

Monday, February 25, 1991

8:30 - 8:45 a.m.	Introductory Remarks - G. Doolen, Los Alamos
- A. Bishop, Los Alamos
8:45 - 9:45 a.m.	"A Physicist looks at Martensites" - J. A. Krumhansl, Cornell U.
	Martensites
Chair - A. Bishop, Los Alamos
9:45 - 10:30 a.m.	"Formation of Martensite in Nickel-Titanium Alloys by Negative Pressure Pulses" - R. B. Schwarz, Los Alamos
10:30 - 10:45 a.m.	Break
10:45 - 11:30 a.m.	"Phonon Anomalies and their Role in First-Order Solid-State Phase Transformations" - L. Tanner, Livermore
11:30 - 12:15 p.m.	"Tweed Precursors in Martensites" - J. Sethna, Cornell U.
12:15 - 1:30 p.m.	Lunch
	Twinning
Chair - R. LeSar, Los Alamos
1:30 - 2:15 p.m.	"Deformation Twinning: Influence of Temperature and Strain Rate" - R. Gray, Los Alamos
2:15 - 3:00 p.m.	"Shapes, Configurations, Stresses and Energies of Twins and Twin Arrays" - T. E. Mitchell, Los Alamos
3:00 - 3:15 p.m.	Break
3:15 - 4:00 p.m.	"Dynamics of Ferroelastic/Martensitic Twinned Structures" - G. Barsch, Penn. State U.
4:00 - 5:00 p.m.	Discussion Leader - A. D. Rollett, Los Alamos
5:15 - 6:15 p.m.	Director's Hosted Reception, Science Museum

Tuesday, February 26, 1991

Fracture

Chair - J. Petrovic, Los Alamos

- 8:30 - 9:15 a.m. "Fragmentation of Films" - R. Cook, Rice U.
- 9:15 - 10:00 a.m. "Fracture of Defected, Brittle Solids" - D. Srolovitz, U. of Michigan
- 10:00 - 10:15 a.m. Break
- 10:15 - 11:00 a.m. "Simple Models for Material Failure and Deformation" - P. Meakin, DuPont
- 11:00 - 11:45 a.m. "Percolation and Failure in Hierarchical Materials" - W. Newman, UCLA/Los Alamos
- 11:45 - 12:15 p.m. "Microstructures in Transformation Toughened Ceramics" - D. Stump, Los Alamos
- 12:15 - 1:30 p.m. Lunch

Stick-Slip

Chair - A. M. Boring

- 1:30 - 2:00 p.m. "Tribological Properties of Structures Formed by Surface Modification Techniques" - M. Nastasi, Los Alamos
- 2:00 - 2:45 p.m. "Interface Contact Area Evolution During Metal Forming" - D. Korzekwa, Los Alamos
- 2:45 - 3:00 p.m. Break
- 3:00 - 3:45 p.m. "Self-Organized Criticality in Stick-Slip Models" - P. Bak, Brookhaven
- 3:45 - 5:30 p.m. Discussion Leader - R. LeSar, Los Alamos
- 6:30 p.m. Dinner (Katherine's)

Wednesday, February 27, 1991

Dislocations

Chair, T. Lowe, Los Alamos

- 8:30 - 9:15 a.m. "Taylor Hardening During Primary and Steady-State Creep in Aluminum and Stainless Steel Alloys" - M. Kassner, Oregon State
- 9:15 - 10:00 a.m. "Structural Instability in High Temperature Plastic Flow" - M. Bocek, Karlsruhe, Germany
- 10:00 - 10:15 a.m. Break
- 10:15 - 11:00 a.m. "Simulation of Dislocation Microstructures During Plastic Flow" - L. Kubin, Paris, France
- 11:00 - 11:45 a.m. "Langevin Molecular Dynamics of Interfaces: Nucleation vs. Spiral Growth" - P. Lomdahl, Los Alamos
- 11:45 - 1:15 p.m. Lunch

Summary Session

Chair, A. D. Rollett, Los Alamos

- 1:15 - 1:45 p.m. "Statistics of Screw Dislocations" - L. Campbell, Los Alamos
- 1:45 - 2:15 p.m. "Opportunities for Lattice Gas Approaches in Materials Modeling" - G. Doolen, Los Alamos
- 2:15 - 3:00 p.m. "Some Problems in Dislocation Kinetics", F. Kocks, Los Alamos
- 3:00 - "Summary Remarks" - J. Krumhansl, Cornell U.

DYNAMICS OF MICROSTRUCTURE WORKSHOP
The Center for Materials Science
and
The Center for Nonlinear Science
February 25-27, 1991

127

F. L. Addessio
Los Alamos National Laboratory
T-3/B216
Los Alamos, NM 87545

Arun K. Bhattacharya
Los Alamos National Laboratory
MST-4/K762
Los Alamos, NM 87545

John Aidun
Los Alamos National Laboratory
T-1/B221
Los Alamos, NM 87545

Alan Bishop
Los Alamos National Laboratory
T-11/B262
Los Alamos, NM 87545

Per Bak
Department of Physics
Brookhaven National Laboratory
Upton, NY 11973

Michael Bocek
Kernforschungszentrum Karlsruhe
Postfach 3640
D-75 Karlsruhe
GERMANY

Gerhard Barsch
107 Materials Research Lab.
Penn State Univ.
University Park, PA 16802

A. M. Boring
Los Alamos National Laboratory
CMS/K765
Los Alamos, NM 87545

Torben Brun
Los Alamos National Laboratory
LANSCE/H805
Los Alamos, NM 87545

Shiyi Chen
Los Alamos National Laboratory
CNLS/B258
Los Alamos, NM 87545

Tim Burke
Los Alamos National Laboratory
CMS/K765
Los Alamos, NM 87545

Shuh-Rong Chen
Los Alamos National Laboratory
CMS/K765
Los Alamos, NM 87545

Larry Campbell
Los Alamos National Laboratory
T-11/B262
Los Alamos, NM 87545

Kim Christensen
Dept. of Physics
Brookhaven National Laboratory
Upton, NY 11973

David Campbell
Los Alamos National Laboratory
CNLS/B258
Los Alamos, NM 87545

Robert Cook
IBM Research Division
T. J. Watson Research Center
Yorktown Heights, NY 10598

Margaret Chadwick
Los Alamos National Laboratory
MST-4/K762
Los Alamos, NM 87545

Ed Cort
Los Alamos National Laboratory
WX-DO/K574
Los Alamos, NM 87545

L. L. Daemen
Los Alamos National Laboratory
T-11/B262
Los Alamos, NM 87545

Jim Gubernatis
Los Alamos National Laboratory
T-11/B262
Los Alamos, NM 87545

Robert J. Donohoe
Los Alamos National Laboratory
INC-4/C345
Los Alamos, NM 87545

Francisco M. Guerra
Los Alamos National Laboratory
WX-11/C931
Los Alamos, NM 87545

Gary Doolen
Los Alamos National Laboratory
CNLS/B258
Los Alamos, NM 87545

James Hammerberg
Los Alamos National Laboratory
X-4/F664
Los Alamos, NM 87545

Joyce A. Goldstone
Los Alamos National Laboratory
LANSCE/H805
Los Alamos, NM 87545

Sun Ig Hong
Los Alamos National Laboratory
MST-5/K762
Los Alamos, NM 87545

Rusty Gray
Los Alamos National Laboratory
MST-5/G730
Los Alamos, NM 87545

Mac Hyman
Los Alamos National Laboratory
T-7/B284
Los Alamos, NM 87545

Loren Jacobson
Los Alamos National Laboratory
MST-6/G770
Los Alamos, NM 87545

Dave A. Korzekwa
Los Alamos National Laboratory
MST-6/G770
Los Alamos, NM 87545

Tom Jervis
Los Alamos National Laboratory
DIR-ESD/A103
Los Alamos, NM 87545

Joel Kress
Los Alamos National Laboratory
T-12/B268
Los Alamos, NM 87545

Kaye A. Johnson
Los Alamos National Laboratory
NMT-5/E506
Los Alamos, NM 87545

James Krumhansl
515 Station Rd.
Amherst, MA 01002

Michael Kassner
Oregon State University
Dept. of Mechanical Engineering
Roger Hall 204
Corvallis, OR 97331-6001

Ladislav Kubin
Lab. d'Etude des Microstructures
CNRS/ONERA (OM)
29, Avenue de la Division Leclerc
B. P. No. 72
F-92322 Chatillon Cedex
FRANCE

Fred Kocks
Los Alamos National Laboratory
CMS/K765
Los Alamos, NM 87545

David Lieberman
Los Alamos National Laboratory
T-11/K765
Los Alamos, NM 87545

Robert Leisure
Los Alamos National Laboratory
CMS/K765
Los Alamos, NM 87545

Michael Nastasi
Los Alamos National Laboratory
MST-7/K765
Los Alamos, NM 87545

Richard LeSar
Los Alamos National Laboratory
T-11/B262
Los Alamos, NM 87545

William Newman
Los Alamos National Laboratory
CNLS/B258
Los Alamos, NM 87545

Peter Lomdahl
Los Alamos National Laboratory
T-11/B262
Los Alamos, NM 87545

Sodano Pasquale
Los Alamos National Laboratory
CNLS/B258
Los Alamos, NM 87545

Paul Meakin
E. I. DuPont de Nemours & Co.
Central Research & Development Dept.
Experimental Station
Wilmington, DE 19898

Dave Phillips
Los Alamos National Laboratory
MST-4/G771
Los Alamos, NM 87545

Terry Mitchell
Los Alamos National Laboratory
CMS/K765
Los Alamos, NM 87545

Roger Pynn
Los Alamos National Laboratory
LANSCE/H805
Los Alamos, NM 87545

Ramon Ravelo
Los Alamos National Laboratory
T-12/B258
Los Alamos, NM 87545

Howard Sizek
Los Alamos National Laboratory
MST-5/K762
Los Alamos, NM 87545

R. A. Robinson
Los Alamos National Laboratory
LANSCE/H805
Los Alamos, NM 87545

Darryl Smith
Los Alamos National Laboratory
MEE-11/D429
Los Alamos, NM 87545

Anthony D. Rollett
Los Alamos National Laboratory
MST-6/K765
Los Alamos, NM 87545

James L. Smith
Los Alamos National Laboratory
ERDC/K763
Los Alamos, NM 87545

Ricardo Schwarz
Los Alamos National Laboratory
CMS/K765
Los Alamos, NM 87545

Steve Spooner
ER132/GTN, MS G236
Division of Materials Science, USDOE
Washington, DC 20585

Jim Sethna
LASSP, Clark Hall
Cornell University
Ithaca, NY 14853

S. Srinivasan
Los Alamos National Laboratory
CMS/K765
Los Alamos, NM 87545

David Srolovitz
Dept. of Materials Science
University of Michigan
Ann Arbor, MI 48109

Davis Tonks
Los Alamos National Laboratory
T-1/B221
Los Alamos, NM 87545

Jim Steele
Los Alamos National Laboratory
NMT-5/E506
Los Alamos, NM 87545

Walter Trela
Los Alamos National Laboratory
P-17/H803
Los Alamos, NM 87545

Timothy S. Sullivan
Los Alamos National Laboratory
P-10/CNLS/B258
Los Alamos, NM 87545

Sam Trickey
Los Alamos National Laboratory
CMS/K765
Los Alamos, NM 87545

David Stump
Los Alamos National Laboratory
MST-6/K765
Los Alamos, NM 87545

Bill Visscher
Los Alamos National Laboratory
T-11/B262
Los Alamos, NM 87545

Lee Tanner
Chemistry & Materials Sci. Tech.
Lawrence Livermore National Lab.
Livermore, CA 94550

Art Voter
Los Alamos National Laboratory
T-12/B268
Los Alamos, NM 87545

Pascal Yvon
Los Alamos National Laboratory
CMS/K765
Los Alamos, NM 87545

Thomas G. Zocco
Los Alamos National Laboratory
MST-5/G730
Los Alamos, NM 87545

JOINT
LOS ALAMOS NATIONAL LABORATORY
AND
SANDIA NATIONAL LABORATORIES
OFFICE OF BASIC ENERGY SCIENCES
MATERIALS SCIENCES INFORMATION AND REVIEW MEETING
MAY 29-30, 1991

Wednesday, May 29, 1991 - J. Robert Oppenheimer Study Center,
TA-3/Bldg. 207, 2nd Floor

- 7:30 a.m. Pick up at Hill Top House.
- 8:00 a.m. Coffee/Registration
- 8:15 a.m. Welcome - Fred Morse, (LANL)
- 8:20 a.m. Introduction - Don Parkin (LANL) and George Samara (SNL)

SESSION I. LOS ALAMOS
Robert H. Heffner, Chairman

- 8:30 a.m. Measuring Residual Strain using Neutrons -
Joyce A. Goldstone and Mark A. M. Bourke.
- 9:00 a.m. Neutron Reflection Studies of Rough Interfaces -
R. Pynn, G. Smith, M. Fitzsimmons, and W. A. Hamilton.
- 9:30 a.m. Probing Chemical Bonds by Neutron Spectroscopy -
Juergen Eckert and G. J. Kubas.
- 10:00 a.m. Magnetic Ordering in Ternary Uranium Compounds -
R. A. Robinson, A. C. Lawson, and K. H. J. Buschow.
- 10:30 a.m. Introduction to Poster Session A - Roger Pynn
- 10:35 a.m. Coffee Break and Poster Session A

POSTER SESSION A (Los Alamos)

1. TiS_2 : A Sponge for Mercury Spills? -
E. W. Ong, J. Eckert, J. A. Goldstone, and R. B. Von Dreele.
2. Neutron Speckle Holography -
D. S. Sivia, G. S. Smith, W. A. Hamilton, and R. Pynn.
3. Microstructure of Composite Materials using Small-Angle Neutron
Scattering and Contrast Variation: Approaches Toward Understanding the
Structure of Carbon Black-Elastomer Mixtures-
Rex P. Hjelm Jr., Wesley A. Wampler, and Philip A. Seeger.

4. Vibrational Spectroscopy of Para-Nitroaniline at High Pressure -
Susanna W. Johnson, Juergen Eckert, Basil I. Swanson, and Joe Thompson.
5. Structural Characterization of Nanocrystalline Pd by X-Ray Diffraction Techniques -
M. R. Fitzsimmons, J. A. Eastman, M. Müller-Stach, and G. Wallner.
6. Understanding Failure in Engineering Components through Non-Destructive Residual Stress Measurements -
Mark A. M. Bourke and Joyce A. Goldstone.
7. High-Temperature Plasticity in Copper Polycrystals -
Shuh Rong Chen and U. F. Kocks.
8. Neutron Irradiation Effects in Bulk and Thin-Film $(\text{Gd,Y})_1\text{Ba}_2\text{Cu}_3\text{O}_{7-x}$ -
K. E. Sickafus, K. M. Hubbard, M. M. Chadwick, S. G. Boeke,
C. J. Salgado, C. D. Kise, F. W. Clinard, Jr., W. A. Coghlan,
K. A. Martin, D. E. Peterson, J. O. Willis, Y. J. Coulter, S. R. Foltyn,
R. C. Dye, R. E. Muenchausen, M. P. Maley, D. M. Parkin, W. B. Wilson,
and G. F. Ramsey.
9. Metastable Phases in Aluminum-Based Intermetallics by Mechanical Alloying -
R. B. Schwarz, S. Srinivasan, and P. Desch.
10. Super-Strong Polymers: Recent Theoretical, Synthesis, and Characterization Results -
F. Dowell.
11. Fracture Behavior of Model SiC-Si₃N₄ Interfaces -
J. J. Petrovic, A. K. Bhattacharya, T. E. Mitchell, and O. Unal.
12. dHvA Effect and Fermi Surface of YBCO -
C. M. Fowler, B. L. Freeman, W. L. Hults, J. C. King, F. M. Mueller,
and J. L. Smith.
13. Synthesis and Characterization of Aromatic Polyamides with Rigid Pendent Chains -
Brian Benicewicz, Thomas Rieker, Marilyn Hawley, and Raimond Liepins.

Video Presentation: Connection Machine Simulation of Spiral Surface Growth: A Langevin Molecular Dynamics Approach
P. S. Lomdahl and A. R. Bishop

12:00 Lunch - Otowi Cafeteria

SESSION II. SANDIA
Tom Picraux, Chairman

- 1:15 p.m. Hydrogen Reactions with Dangling Bonds in Si and Si-SiO₂ Structures -
S. M. Myers, K. L. Brower, D. M. Follstaedt, P. M. Richards,
H. J. Stein, and W. R. Wampler.
- 1:45 p.m. Transport and Pinning in High Quality Tl-Ca-Ba-Ca-O Films -
D. S. Ginley, E. L. Venturini, C. P. Tigges,
T. E. Zipperian, J. C. Barbour, and B. Morosin.
- 2:15 p.m. The Interfacial Transition Region in Ultra-Thin Overlayer Systems -
J. E. Houston and N. D. Shinn.
- 2:45 p.m. Layer-by-Layer Sputtering of Silicon -
P. Bedrossian, T. Klitsner, E. Chason, J. E. Houston,
J. Y. Tsao, and S. T. Picraux.
- 3:15 p.m. Introduction to Poster Session B - George Samara
- 3:20 p.m. Coffee Break and Poster Session B

• POSTER SESSION B (Sandia)

1. New Nonlinear Optical Ceramics Through Ion Exchange of KTiOPO₄ and KTiOAsO₄ -
M. Phillips.
2. Metal-Oxide/Metal Interfaces: A Surface Science Approach to the Study of Adhesion -
C. H. F. Peden, N. D. Shinn, and K. B. Kidd
3. Micromechanics of Adhesive Contact -
P. A. Taylor, J. S. Nelson, and B. W. Dodson.
4. Interfacial Forces at Metal/Insulator Surfaces: Role of Charge Transfer -
S. Joyce, J. E. Houston, and T. A. Michalske.
5. Site Specific Chemistry on Semiconductor Surfaces -
T. Klitsner and J. S. Nelson.
6. Enhanced Tribology of Ion-Implanted Aluminum -
M. T. Dugger, R. J. Bourcier, D. M. Follstaedt, and S. M. Myers.
7. Low Temperature Synthesis of Si₃N₄ Films in ECR Plasmas -
J. C. Barbour and H. J. Stein.

8. Atomic Mechanisms for Diffusion of Single Atoms and Small Clusters on Metal Surfaces -
G. L. Kellogg.
9. Modeling Si Surface Sputtering and Growth Dynamics -
E. Chason and B. W. Dodson.
10. Structure and Bonding in Boron Carbides -
D. Emin, T. L. Aselage, and B. Morosin.
11. Effect of Strain- and Alloy-Fluctuations on the Electron Mobility in Lattice-Matched and Strained Ternary Quantum Wells-
S. K. Lyo and I. J. Fritz.
12. Effective Masses in Compound Semiconductor Quantum Wells -
E. Jones.
13. Experimental Studies of CVD Kinetics -
P. Ho and K. P. Killeen.
14. Numerical Modeling of Kinetics in CVD -
M. E. Coltrin.
15. Pressure Induced Record-High Transition Temperature Organic Superconductors -
J. E. Schirber, B. L. Overmyer, H. H. Wang, and J. M. Williams.
16. Annealing and Structural Studies of Tl-Ca-Ba-Cu-O Superconductors -
E. L. Venturini, B. Morosin, D. S. Ginley, R. J. Baughman, C. P. Tigges, and M. A. Mitchell.
17. Complex Powder Compressibility -
A. J. Hurd, D. M. Smith (UNM), and P. Seeger (LANL).
18. High Temperature Phase Equilibria in Thallium-Containing High T_c Superconductors -
T. L. Aselage, E. L. Venturini, J. A. Voigt, and T. J. Headley.

Video Presentation: Modeling Si Surface Sputtering and Growth Dynamics -
E. Chason and B. W. Dodson.

5:15 p.m. Director Hosted Reception - J. Robert Oppenheimer Study Center

6:30 p.m. Dinner - Otowi Building

7:30 p.m. Transportation to Hill Top House

Thursday, May 30, 1991

SESSION III. SANDIA
Ron Loehman (Chairman)

- 7:30 a.m. Pick up at Hill Top House.
- 8:00 a.m. Coffee/Registration
- 8:20 a.m. Capillary Phenomena in Sol-Gel Film Formation -
C. J. Brinker and A. J. Hurd.
- 8:45 a.m. Semiconductor Interface Modification by Strain and Dipoles -
J. S. Nelson.
- 9:10 a.m. Vibrational Spectra of Icosahedral Borides -
D. R. Tallant, T. L. Aselage, and D. Emin.
- 9:35 a.m. Surface Chemistry of GaAs MOCVD -
J. R. Creighton.
- 10:00 a.m. Coffee Break

SESSION IV. LOS ALAMOS
Don Parkin, Chairman

- 10:30 a.m. An Interatomic Potential for Directional Bonding: The Rotated
Second Moment Approximation -
Arthur F. Voter and Joel D. Kress.
- 10:55 a.m. Growth Mechanism and High T_c Films as Studied by Scanning
Tunneling and Atomic Force Microscopies -
M. E. Hawley, R. Dye, S. R. Foltyn, R. E. Muenchausen,
Ian Raistrick, Robert Houlton, and X. D. Wu.
- 11:20 a.m. NMR Studies of the High Temperature Superconductors $YBa_2Cu_3O_{7-y}$ -
P. C. Hammel.
- 11:45 a.m. Fracture Toughness as a Function of Phase Angle of an
Alumina/Niobium Interface -
M. G. Stout, N. P. O'Dowd, C. F. Shih, R. J. Asaro.
- 12:10 p.m. Lunch - Otowi Building
- 1:30 p.m. LANSCE Facility Tour - R. Pynn or
Individual arranged visits.

Transportation from J. Robert Oppenheimer Study Center to the Hilltop
House Hotel.

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MATERIALS SCIENCE INFORMATION AND REVIEW
MEETING
MAY 29 - 30, 1991
J. ROBERT OPPENHEIMER STUDY CENTER

Al J. Arko
Los Alamos National Laboratory
P-10
Mailstop K764
Los Alamos, NM 87545

John Charles Barbour
Sandia National Laboratories
Division 1111, MS 1112
Albuquerque, NM 87185

Robert J. Asaro
Los Alamos National Laboratory
MST-5
Mailstop G770
Los Alamos, NM 87545 .

Peter J. Bedrossian
Sandia National Laboratories
Division 1114
Albuquerque, NM 87185-5800

Terrence L. Aselage
Sandia National Laboratories
Division 1842
Albuquerque, NM 87185

Brian C. Benicewicz
Los Alamos National Laboratory
MST-7
Mailstop E549
Los Alamos, NM 87545

Larry R. Austin
Los Alamos National Laboratory
NMT-2
Mailstop E501
Los Alamos, NM 87545

Howard K. Birnbaum
Univ. of Illinois
Materials Research Lab.
104 So. Goodwin Ave.,
Urbana, IL 61801

Alan R. Bishop
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

Otto Buck
Ames Laboratory
Iowa State University
Ames, IA 50011

Larry S. Blair
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

Torben Brun
Los Alamos National Laboratory
LANSCE
Mailstop H805
Los Alamos, NM 87545

A. M. Boring
Los Alamos National Laboratory
Center for Materials Science
Mailstop K765
Los Alamos, NM 87545

Hugh Casey
Los Alamos National Laboratory
ADCM
Mailstop K763
Los Alamos, NM 87545

Mark A. Bourke
Los Alamos National Laboratory
LANSCE
Mailstop H805
Los Alamos, NM 87545

Eric Chason
Sandia National Laboratories
Division 1111
Albuquerque, NM 87185

C. Jeffrey Brinker
Sandia National Laboratories
Division 1846
Albuquerque, NM 87185-5800

Daniel S. Chemla
Lawrence Berkeley Laboratory
MS-66
1 Cyclotron Road
Berkeley, CA 94720

Shao-Ping Chen
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos NM 87545

Art Denison
EG&G Idaho Inc.
P.O. Box 1625
Idaho Falls, ID 83415-2211

Shuh-Rong Chen
Los Alamos National Laboratory
Center for Materials Science
Mailstop K765
Los Alamos, NM 87545

Paul B. Desch
Los Alamos National Laboratory
Center for Materials Science
Mailstop K765
Los Alamos, NM 87545

Albert M. Clogston
Los Alamos National Laboratory
Center for Materials Science
Mailstop K765
Los Alamos, NM 87545

Robert J. Donohoe
Los Alamos National Laboratory
INC-4
Mailstop C345
Los Alamos, NM 87545

Michael E. Coltrin
Sandia National Laboratories
Division 1126
Albuquerque, NM 87185

Flonnie Dowell
Los Alamos National Laboratory
T-12
Mailstop B268
Los Alamos, NM 87545

J. Randall Creighton
Sandia National Laboratories
Division 1126
Albuquerque, NM 87185-5800

Barney L. Doyle
Sandia National Laboratories
Division 1111
Albuquerque, NM 87185-5800

Michael T. Dugger
Sandia National Laboratories
Division 1832
Albuquerque, NM 87185-5800

Gregory J. Exarhos
Pacific Northwest Laboratory
P. O. Box 999
MS K2-44
Richland, WA 99352

Bob D. Dunlap
Argonne National Laboratory - 212
9700 S. Cass Avenue
Argonne, IL 60439

Michael R. Fitzsimmons
Los Alamos National Laboratory
LANSCE
Mailstop H805
Los Alamos NM 87545

Robert C. Dye
Los Alamos National Laboratory
CLS-2
Mailstop K763
Los Alamos, NM 87545

Paul Follansbee
Los Alamos National Laboratory
MST-DO
Mailstop G756
Los Alamos, NM 87545

Juergen Eckert
Los Alamos National Laboratory
LANSCE
Mailstop H805
Los Alamos, NM 87545

Stephen R. Foltyn
Los Alamos National Laboratory
CLS-6
Mailstop K763
Los Alamos, NM 87545

David Emin
Sandia National Laboratories
Division 1152
Albuquerque, NM 87185

Clarence Maxwell Fowler
Los Alamos National Laboratory
M-6
Mailstop J970
Los Alamos, NM 87545

Frank D. Gac
Los Alamos National Laboratory
MST-4
Mailstop G771
Los Alamos, NM 87545

John C. Hamilton
Sandia National Laboratories
Division 8342
Livermore, CA 94550

James B. Gerardo
Sandia National Laboratories
Division 1120
Albuquerque, NM 87185-5800

P. Chris Hammel
Los Alamos National Laboratory
P-10
Mailstop K764
Los Alamos, NM 87545

David S. Ginley
Organization 1144
Sandia National Laboratories
Albuquerque, NM 87185-5800

Marilyn E. Hawley
Los Alamos National Laboratory
MST-7
Mailstop E549
Los Alamos, NM 87545

Joyce A. Goldstone
Los Alamos National Laboratory
LANSCE
Mailstop H805
Los Alamos, NM 87545

Robert H. Heffner
Los Alamos National Laboratory
P-10
Mailstop K764
Los Alamos, NM 87545

Rueben L. Gutierrez
Los Alamos National Laboratory
NMT-5
Mailstop E506
Los Alamos, NM 87545

Rex Hjelm
Los Alamos National Laboratory
LANSCE
Mailstop H805
Los Alamos, NM 87545

Pauline Ho
Sandia National Laboratories
Division 1126
Albuquerque, NM 87185-5800

Alan Hurd
Sandia National Laboratories
Division 1841
Albuquerque, NM 87185-5800

Linda L. Horton
Metals and Ceramics Division
Oak Ridge National Laboratory
P. O. Box 2008
Oak Ridge, TN 37831-6118

Reed J. Jensen
Los Alamos National Laboratory
ADCM
Mailstop A102
Los Alamos, NM 87545

Jack E. Houston
Sandia National Laboratories
Division 1114
P. O. Box 5800
Albuquerque, NM 87185

A. Wayne Johnson
Sandia National Laboratories
Division 1126
Albuquerque, NM 87185-5800

John Y. Huang
Los Alamos National Laboratory
NMT-9
Mailstop E502
Los Alamos, NM 87545

Susanna W. Johnson
Los Alamos National Laboratory
LANSCE
Mailstop H805
Los Alamos, NM 87545

W. Larry Hults
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

Eric D. Jones
Sandia National Laboratories
Division 1143
Albuquerque, NM 87185-5800

Andrew S. Jordan
AT&T Bell Laboratories
600 Mountain Avenue
Room 7D-414
Murray Hill, NJ 07974

U. Fred Kocks
Los Alamos National Laboratory
Center for Materials Science
Mailstop K765
Los Alamos, NM 87545

Stephen A. Joyce
Sandia National Laboratories
Division 1112
Albuquerque, NM 87185-5800

Jun-Ichi Koike
Los Alamos National Laboratory
Center for Materials Science
Mailstop K765
Los Alamos, NM 87545

Richard D. Kelley
Division of Materials Sciences
ER-132
U. S. Department of Energy
Washington, DC 20585

Joel D. Kress
Los Alamos National Laboratory
T-12
Mailstop B268
Los Alamos, NM 87545

Gary L. Kellogg
Sandia National Laboratories
Division 1114
Albuquerque, NM 87185-5800

Angus C. Lawson
Los Alamos National Laboratory
MST-5
Mailstop G730
Los Alamos, NM 87545

Tom Klitsner
Sandia National Laboratories
Division 1111
Albuquerque, NM 87185-5800

Ross Lemons
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

Richard A. LeSar
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

Terry C. Lowe
Los Alamos National Laboratory
MST-5
Mailstop G730
Los Alamos, NM 87545

Raimond Liepins
Los Alamos National Laboratory
MST-7
Mailstop E549
Los Alamos, NM 87545

Sungkwun K. Lyo
Sandia National Laboratories
Division 1143
Albuquerque, NM 87185-5800

Xuan Liu
Los Alamos National Laboratory
LANSCE
Mailstop H805
Los Alamos, NM 87545

Stuart R. MacEwen
Alcan International Limited
Kingston Research & Dev. Centre
945 Princess St.
P. O. Box 8400
Kingston, Ontario
CANADA K7L 5L9

Ronald E. Loehman
Sandia National Laboratories
Department 1840
Albuquerque, NM 87185

George Mah
EG&G Rocky Flats, Inc.
Rocky Flats Plant
P. O. Box 464
Golden, CO 80403-0464

Peter S. Lomdahl
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

Terry A. Michalske
Sandia National Laboratories
Division 1114
Albuquerque, NM 87185-5800

Terence E. Mitchell
Los Alamos National Laboratory
Center for Materials Science
Mailstop K765
Los Alamos, NM 87545

Ross E. Muenchausen
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

Harry K. Moffat
Sandia National Laboratories
Division 1126
Albuquerque, NM 87185-5800

Samuel M. Myers
Sandia National Laboratories
Division 1112
Albuquerque, NM 87185-5800

Bruno Morosin
Sandia National Laboratories
Albuquerque, NM 87185-5800

Jeff Nelson
Sandia National Laboratories
Division 1143
Albuquerque, NM 87185-5800

Fred Morse
Los Alamos National Laboratory
ADR
Mailstop A114
Los Alamos, NM 87545

Eddie W. Ong
Los Alamos National Laboratory
LANSCE
Mailstop H805
Los Alamos, NM 87545

Fred M. Mueller
Los Alamos National Laboratory
Center for Materials Science
Mailstop K765
Los Alamos, NM 87545

John A. Panitz
The University of New Mexico
Department of Physics & Astronomy
800 Yale Blvd
Albuquerque, NM 87131

Don M. Parkin
Los Alamos National Laboratory
Center for Materials Science
Mailstop K765
Los Alamos, NM 87545

Roger Pynn
Los Alamos National Laboratory
LANSCE
Mailstop H805
Los Alamos, NM 87545

Charles H. F. Peden
Sandia National Laboratories
1846
Albuquerque, NM 87185-5800

Dwight G. Rickel
Los Alamos National Laboratory
M-6
Mailstop J970
Los Alamos, NM 87545

John J. Petrovic
Los Alamos National Laboratory
MST-4
Mailstop G771
Los Alamos, NM 87545

Jeanne M. Robinson
Los Alamos National Laboratory
CLS-4
Mailstop J567
Los Alamos, NM 87545

Mark L. F. Phillips
Sandia National Laboratories
Division 1845
Albuquerque, NM 87185

Robert A. Robinson
Los Alamos National Laboratory
LANSCE
Mailstop H805
Los Alamos, NM 87545

Samuel T. Picraux
Sandia National Laboratories
Division 1110
Albuquerque, NM 87185-5800

Anthony D. Rollett
Los Alamos National Laboratory
MST-6
Mailstop G770
Los Alamos, NM 87545

James A. Salsgiver
Tech CTR
Allegheny Ludlum Corporation
Brackenridge, PA 15014

Ricardo B. Schwarz
Los Alamos National Laboratory
Center for Materials Science
Mailstop K765
Los Alamos, NM 87545

George A. Samara
Sandia National Laboratories
Division 1150
Albuquerque, NM 87185-5800

Neal D. Shinn
Sandia National Laboratories
Division 1114
Albuquerque, NM 87185-5800

Alfred P. Sattelberger
Los Alamos National Laboratory
INC-DO
Mailstop J515
Los Alamos, NM 87545

Kurt E. Sickafus
Los Alamos National Laboratory
MST-4
Mailstop K762
Los Alamos, NM 87545

David Schiferl
Los Alamos National Laboratory
M-6
Mailstop C345
Los Alamos, NM 87545

David C. Smith
Los Alamos National Laboratory
INC-4
Mailstop C346
Los Alamos, NM 87545

James E. Schirber
Sandia National Laboratories
Division 1090
Albuquerque, NM 87185-5800

Gregory S. Smith
Los Alamos National Laboratory
LANSCE
Mailstop H805
Los Alamos, NM 87545

James L. Smith
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

Galen K. Straub
Los Alamos National Laboratory
T-1
Mailstop B221
Los Alamos, NM 87545

Steve Spooner
U. S. DOE/DMS
ER-132/GTN
MS G236
Division of Materials Sciences
U.S. DOE
Washington, DC 20485

David R. Tallant
Sandia National Laboratories
Division 1821
Albuquerque, NM 87185-5800

Sreeram Srinivasan
Los Alamos National Laboratory
Center for Materials Science
Mailstop K765
Los Alamos, NM 87545

Paul A. Taylor
Sandia National Laboratories
Division 1153
Albuquerque, NM 87185-5800

Eugene E. Stark
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

Thomas N. Taylor
Los Alamos National Laboratory
CLS-2
Mailstop G738
Los Alamos, NM 87545

Michael G. Stout
Los Alamos National Laboratory
MST-5
Mailstop G730
Los Alamos, NM 87545

Eugene L. Venturini
Sandia National Laboratories
Division 1152
Albuquerque, NM 87185-5800

Frederick L. Vook
Sandia National Laboratories
Organization 1100
Albuquerque, NM 87185-5800

Xin Di Wu
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

Arthur F. Voter
Los Alamos National Laboratory
T-12
Mailstop B268
Los Alamos, NM 87545

Pascal J. Yvon
Los Alamos National Laboratory
Center for Materials Science
Mailstop K765
Los Alamos, NM 87545

Steven R. Walter
Rocky Flats Plant
Building 779
P.O. Box 464
Golden, CO 80402-0464

Alan D. Wilks
Allied Signal
50 East Algonquin Road
2 Plaines, IL 60017

W. G. Wolfer
Sandia National Laboratories
Livermore, CA 94550

INCOR Meeting Agenda
 Otowi Building, Cafeteria Rooms B & C
 Los Alamos National Laboratory
 April 26, 1991

RECEPTION - Thursday, April 25, 1991

7:30 p.m. - 9:00 p.m., Los Alamos Inn, Jemez Room

Friday, April 26, 1991, Otowi Building, Cafeteria Rooms B & C

8:45 a.m. - 8:50 a.m. A. Bishop, LANL
 "Introduction"

8:50 a.m. - 9:40 a.m. Z. Fisk, LANL
 "Experimental Overview"

9:40 a.m. - 10:05 a.m. C. Almasan, UCSD [M. Maple, Z. Fisk, S.-H. Han]
 "Pressure Dependence of T_c of Oxygen Deficient
 $YBa_2Cu_3O_x$ "

10:05 a.m. - 10:30 a.m. O. Klein, UCLA [G. Gruner, Z. Fisk]
 "Conductivity Coherence Peaks in Superconducting
 Oxides"

10:30 a.m. - 10:45 a.m. Break

10:45 a.m. - 11:10 a.m. G. Zimanyi, UCD [K. Bedell]
 "Scaling Theory of Marginal Fermi Liquids"

11:10 a.m. - 11:35 a.m. S.-Q. Lu, UCSD [L. Sham, K. Bedell]
 "Heavy Hole in a Metallic Host"

11:35 a.m. - 12:00 noon M. Smith, UCSD & UT [H. Oesterreicher, D. Taylor]
 "Transition-Metal Site Occupancy and Crystal
 Structure in $YBa_2Cu_3O_{6+y}$ "

12:00 noon - 12:25 p.m. A. Heeger, UCSB [J. Thompson, G. Yu]
 " "

12:25 p.m. - 1:30 p.m. Lunch

1:30 p.m. - 2:20 p.m. K. Bedell, LANL
 "Theoretical Overview"

2:20 p.m. - 2:45 p.m. A. Portis, UCB [W. Cooke]
 "Microwave Surface Impedance Studies of the
 High-Temperature Superconductors"

2:45 p.m. - 3:10 p.m. K. Bennett and F. Heidelbach, UCB [R. Wenk,
 T. Rollett]
 "Texture Analysis of High Temperature Superconductors
 with X-Ray and Neutron Diffraction"

INCOR Meeting Agenda, Continued
April 26, 1991

- 3:10 p.m. - 3:25 p.m. Break
- 3:25 p.m. - 3:50 p.m. A. Reyes, UCR & LANL [D. MacLaughlin, R. Heffner]
"NMR Studies in $Y_{1-x}Pr_xBa_2Cu_3O_7$ "
- 3:50 p.m. - 4:15 p.m. J. Shi, UCLA [R. Bruinsma, A. Bishop]
"Polarons in MX Chain Compounds"
- 4:15 p.m. - 4:40 p.m. M. Steiner, UCSD [L. Sham, R. Albers]
"Perturbation Theory of Correlated Systems: A Model System and a Real System"
- 4:40 p.m. - 5:05 p.m. E. Ahrens, UCLA [W. Clark, R. Heffner]
"Heavy Fermion NMR"
- 5:30 p.m. - 7:00 p.m. Steering Committee Meeting
Location to be announced

HTC INCOR MEETING

Los Alamos, NM

April 26, 1991

Eric Ahrens
Los Alamos National Laboratory
P-10
Mailstop K764
Los Alamos, NM 87545

Kristin Bennett
Dept. of Geology & Geophysics
UC Berkeley
Berkeley, CA 94720

Bob Albers
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

Alan R. Bishop
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

Carmen Almasan
UC San Diego
IPAPS-0075
9500 Gilman Drive
La Jolla, CA 92093-0075

Larry Campbell
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

Kevin S. Bedell
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

D. Wayne Cooke
Los Alamos National Laboratory
MP-14
Mailstop H844
Los Alamos, NM 87545

Zack Fisk
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Olivier Klein
Department of Physics
UC Los Angeles
405 Hilgard Ave.
Los Angeles, CA 90024

George Gruner
Dept. of Physics
UC, Los Angeles
405 Hilgard Ave
Los Angeles, CA 90024-1595

Shi-Qin Lu
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

Alan Heeger
Department of Physics
UC Santa Barbara
Santa Barbara, CA 93106

M. Brian Maple
Department. of Physics - 0319
UC San Diego
9500 Gilman Drive
La Jolla, CA 92093-0319

Robert H. Heffner
Los Alamos National Laboratory
P-10
Mailstop K764
Los Alamos, NM 87545

Jose Mustre-de-Leon
Los Alamos National Laboratory
MEE-11
Mailstop D429
Los Alamos, NM 87545

Florian Heidelbach
Dept. of Geology and Geophysics
UC Berkeley
Berkeley, CA 94720

John Oesterreicher
Department of Chemistry, 0317
UC San Diego
9500 Gilman Drive
La Jolla, CA 92093-0317

Alan M. Portis
Department of Physics
UC Berkeley
Berkeley, CA 94720

Matthew Steiner
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

Arneil P. Reyes
Los Alamos National Laboratory
P-10
Mailstop K764
Los Alamos, NM 87545

R. Dean Taylor
Los Alamos National Laboratory
P-10
Mailstop K764
Los Alamos, NM 87545

A. D. Rollett
Los Alamos National Laboratory
MST-6
Mailstop G770
Los Alamos, NM 87545

Joe D. Thompson
Los Alamos National Laboratory
P-10
Mailstop K764
Los Alamos, NM 87545

Michael Smith
The University of Texas at Austin
Center for Materials Science and Eng.
ETC 9.104
Austin, TX 78712

Rudy Wenk
Dept. Geology and Geophysics
UC Berkeley
Berkeley, CA 94720

Jia Shi
Department of Physics
UC Los Angeles
Los Angeles, CA 90024

Gergely Zimanyi
Department of Physics
UC Davis
Davis, CA 95616

Los Alamos Workshop on PROCESS MODELLING IN MATERIALS

Monday, 5 August 1991: Oppenheimer Study Center

Chair: John Hirth

8:30 Coffee

9:00 Don Parkin: Welcome

9:10 Mike Ashby: Proper Planning of Modelling Activities

10:10 Fred Kocks: Dealing with Complexity

11:10 Bob Schaefer: Application of Process Modelling to Intelligent Processing of Materials (IPM) - HIP

11:30 DISCUSSION

11:50 Lunch - go through line at Otowi Cafeteria then proceed to Side Room B

Chair: Frans Spaepen

13:30 Keith Brimacombe: The Modelling of Casting Processes for Quality Improvements

14:10 DISCUSSION

14:30 Tony Hirt: Modelling Fluid Flow

14:50 DISCUSSION

15:10 Break

15:40 Julian Szekely: Modelling Welding

16:20 DISCUSSION

16:40 Artie Ortega: Aspects of the Numerical Modelling of Welding Processes

17:00 DISCUSSION

17:30 Director's Reception

Tuesday, 6 August 1991: Fuller Lodge**Chair: Dave Clarke****8:30 Paul Follansbee: Modelling Plasticity****9:10 DISCUSSION****9:30 Jim Johnson: Modelling Shock Fronts****9:50 DISCUSSION****10:10 Break****10:40 Mike Stout: Data Acquisition, Anisotropy****11:10 DISCUSSION****11:30 Paul Maudlin: Sensitivity of FEM Results to Microscale Models****12:00 DISCUSSION**

12:20 Vans to Ski Lodge for Catered Lunch (\$5.00)

Chair: Hugh Casey**15:00 Paul Dawson: Microscale Models for Macroscale Processes****15:40 DISCUSSION****16:00 Bert Van Bael: Finite Element Modelling of Anisotropic Plasticity****16:20 DISCUSSION****16:40 Dave Korzekwa: Modelling Friction****17:00 DISCUSSION****17:20 Stuart MacEwen: Modelling and Validation of Sheet Metal Forming****18:00 DISCUSSION**

Wednesday, 7 August 1991: Fuller Lodge

Chair: Mike Luton

8:30 Mike Sellars: High-Temperature Forming

9:10 DISCUSSION

9:30 Larry Lalli: Modelling and Validation of Fabrication Processes

9:50 DISCUSSION

10:10 Break

10:40 Hugh Shercliff: Modelling Age-Hardening

11:00 DISCUSSION

11:20 Roger Doherty: Modelling Structure Change

12:00 DISCUSSION

12:20 Catered Lunch at Fuller Lodge (\$5.00)

Chair: Ron Scattergood

13:30 Doug Bammann: Damage Modelling in Materials Processing

13:50 DISCUSSION

14:10 Jean LeMaitre: Thermodynamical Modelling of Viscoplastic Strain, Damage,
Phase Transformations and their Couplings

14:50 DISCUSSION

15:10 Break

15:40 Dave Embury: Experimental Verification of Models, with Examples

16:00 DISCUSSION

16:20 Rudy Wenk: Modelling the Past

17:00 DISCUSSION

17:30 Vans to Picnic at Sportman's Park (\$10.00)

Thursday, 8 August 1991: Fuller Lodge

Chair: Dave Embury

8:30 Tony Rollett: Process Modelling Needs

9:15 Terry Lowe: Properties Modelling Needs

10:00 Break

10:30 EXTENDED DISCUSSION

11:20 Karl-Heinz Winkler: Computer Opportunities

11:40 DISCUSSION

12:00 Group Lunch at Pizza Hut (\$5.00)

Chair: Mike Baskes

13:00 Richard LeSar: Atomistic Modelling Capabilities

13:40 Brad Holian: Molecular Dynamics

14:00 DISCUSSION

14:20 Coffee

14:50 Bob Asaro: Instabilities Physical and Computational

15:30 DISCUSSION

15:50 Heinz Mecking: Overall Assessment

16:30 Adjourn

WORKSHOP ON
PROCESS MODELLING IN MATERIALS

Los Alamos National Laboratory
Los Alamos, NM 87545
August 5 - 8, 1991

LIST OF PARTICIPANTS

Said Ahzi
University of California, San Diego
Dept. Applied Mech. & Eng. Sci.
La Jolla, CA 92093

Prof. Michael Ashby
University Eng. Dept.
Trumpington Street
Cambridge CB2 1P2
UNITED KINGDOM

Allan Anderson
Los Alamos National Laboratory
M-9
Mailstop P952
Los Alamos, NM 87545

Michael Baskes
U.S. Department of Energy
Division of Materials Sciences
ER-131/GTN
Washington, DC 20585

Harry Armen
Jeff Bingamen, U.S. Senators Office
524 Hart Building
Washington, DC 20510

Dr. Lee Bertram
Sandia Livermore
P.O. Box 969
Org. 8243 Bldg. 912
Livermore, CA 94550

Prof. Robert Asaro
University of California, San Diego
Dept. Applied Mech. & Eng. Sci.
La Jolla, CA 92093

Arun Bhattacharya
Los Alamos National Laboratory
MST-4
Mailstop K762
Los Alamos, NM 87545

Prof. Keith Brimacombe
University of British Columbia
Dept. of Metallurgical Eng.
Vancouver, BC
CANADA V6T 1W5

Edward Cort
Los Alamos National Laboratory
WX-DO
Mailstop K574
Los Alamos, NM 87545

Hugh Casey
Los Alamos National Laboratory
ADCM
Mailstop K763
Los Alamos, NM 87545

Prof. Paul Dawson
Cornell University
Mechanical & Aerospace Eng.
Ithaca, NY 14853

Shao Ping Chen
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

Jerry Dick
Los Alamos National Laboratory
M-9
Mailstop P952
Los Alamos, NM 87545

Shuh-Rong Chen
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Gary Dilts
Los Alamos National Laboratory
X-4
Mailstop F664
Los Alamos, NM 87545

Professor David R. Clarke
Univ. California, Santa Barbara
Materials Department
Santa Barbara, CA 93106

Prof. Roger Doherty
Drexel University
Dept. Materials Eng.
Philadelphia, PA 19104

Prof. J. David Embury
McMaster University
Materials Science & Eng. Dept.
Hamilton ON L8S 4L7
CANADA

Kenneth Hanson
Los Alamos National Laboratory
M-4
Mailstop P940
Los Alamos, NM 87545

Dr. Elane O. Flower
Lawrence Livermore National Lab.
L-342
Livermore, CA 94550

Florian Heidelberg
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Paul Follansbee
Los Alamos National Laboratory
MST-DO
Mailstop G756
Los Alamos, NM 87545

C. W. (Tony) Hirt
Flow Science, Inc.
P.O. Box 933
1325 Trinity Dr.
Los Alamos, NM 87544

Jeffery C. Gibeling
University of California, Davis
Dept. of Mechanical Eng.
Davis, CA 95616

Prof. John Hirth
Washington State University
Mechanical & Materials Eng.
Pullman, WA 99164

George T. (Rusty) Gray III
Los Alamos National Laboratory
MST-5
Mailstop G730
Los Alamos, NM 87545

Brad Holian
Los Alamos National Laboratory
T-12
Mailstop B268
Los Alamos, NM 87545

Kathleen S. Holian
Los Alamos National Laboratory
C-9
Mailstop B295
Los Alamos, NM 87545

David Korzekwa
Los Alamos National Laboratory
MST-6
Mailstop G770
Los Alamos, NM 87545

Elizabeth Holm
Los Alamos National Laboratory
MST-6
Mailstop G770
Los Alamos, NM 87545

Deniece Korzekwa
Los Alamos National Laboratory
MST-6
Mailstop G770
Los Alamos, NM 87545

James N. Johnson
Los Alamos National Laboratory
T-1
Mailstop B221
Los Alamos, NM 87545

Joel Kress
Los Alamos National Laboratory
T-12
Mailstop B268
Los Alamos, NM 87545

Kaye Johnson
Los Alamos National Laboratory
NMT-5
Mailstop E506
Los Alamos, NM 87545

Prof. Veli Tapani Kuokkala
Tampere Univ. of Tech. Materials Scie
P.O. Box 527
SF-33101
Tampere, FINLAND

Fred Kocks
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Pang-Jen Kung
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

Dr. Larry Lalli
ALCOA Tech. Center
Alcoa, PA 15069

Mary Ann Lewis
Los Alamos National Laboratory
WX-11
Mailstop C931
Los Alamos, NM 87545

Sam Lambrakos
Naval Research Laboratory
Materials Science Division
Code 6324
Washington, DC 20375-5000

David S. Lieberman
Los Alamos National Laboratory
T-11
Mailstop K765
Los Alamos, NM 87545

Henry Laquer
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

Terry Lowe
Los Alamos National Laboratory
MST-5
Mailstop G730
Los Alamos, NM 87545

Prof. Jean LeMaitre
LMT, Univ. Paris 6
61 Av. du Pres. Wilson
94230 Cachan
FRANCE

Dr. Michael Luton
EXXON Research & Eng. Co.
Route 22 East
Annandale, NJ 08801

Richard LeSar
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

Dr. Stuart MacEwen
Alcan Research Center
Kingston, Ontario
CANADA K7L 424

David Mandell
Los Alamos National Laboratory
X-3
Mailstop F663
Los Alamos, NM 87545

Thanasis Papathanasiou
Los Alamos National Laboratory
MEE-4
Mailstop G787
Los Alamos, NM 87545

Paul Maudlin
Los Alamos National Laboratory
N-6
Mailstop K557
Los Alamos, NM 87545

Don M. Parkin
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Prof. Dr. Heinz Mecking
Techn. Univ. Hamburg-Harburg
Postfach 901403
21 Hamburg 90
GERMANY

Warren Poole
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos NM 87545

Daniel J. Nikkel, Jr.
Lawrence Livermore National Lab.
P.O. Box 808
L-342
Livermore, CA 94550

Dr. Marek Przystupa
UC, Los Angeles
Dept. of Materials Science & Eng.
5731 Boelter Hall
Los Angeles, CA 90024

Dr. Artie Ortega
Sandia National Laboratories
Org. 8244
Bldg. 912
Livermore, CA 94550

A. D. (Tony) Rollett
Los Alamos National Laboratory
MST-6
Mailstop G770
Los Alamos, NM 87545

Dr. Ron O. Scattergood
North Carolina State University
Dept. of Materials Eng.
Raleigh, NC 27607

Ricardo B. Schwarz
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Dr. Robert J. Schaefer
NIST
Materials Division
Gaithersburg, MD 20899

Prof. C. M. Sellars
The University of Sheffield
School of Materials
Sheffield S1 3JD
ENGLAND

Sheila Schiferl
Los Alamos National Laboratory
N-6
Mailstop K557
Los Alamos, NM 87545

Anthony Sgro
Los Alamos National Laboratory
X-3
Mailstop F663
Los Alamos, NM 87545

Richard W. Schmude
Los Alamos National Laboratory
NMT-1
Mailstop E505
Los Alamos, NM 87545

Dr. Hugh Shercliff
Univ. Engineering Dept.
Trumpington St.
Cambridge, CB2 1PZ
ENGLAND

Larry Schwalbe
Los Alamos National Laboratory
X-3
Mailstop F663
Los Alamos, NM 87545

Howard Sizek
Los Alamos National Laboratory
MST-5
Mailstop K762
Los Alamos, NM 87545

Prof. Frans Spaepen
Harvard University
Applied Science Dept.
Cambridge, MA 02138

Naresh N. Thadhani
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Sreeram Srinivasan
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Dr. Robb Thomson
NIST
Materials Research Center
Washington, DC 20234

James H. Steele, Jr.
Los Alamos National Laboratory
NMT-5
Mailstop E506
Los Alamos, NM 87545

Dr. Bert Van Bael
MTM, KUL
deCroylan 2
3030 Leuven
BELGIUM

Michael Stout
Los Alamos National Laboratory
MST-5
Mailstop G730
Los Alamos, NM 87545

Bill Visscher
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

Prof. Julian Szekeley
MIT 4-117
Dept. Materials Science & Eng.
Cambridge, MA 02139

Branimir F. von Turkovich
NSF
1800 G. St. N.W. #1128
Washington, DC 20550

Art Voter
Los Alamos National Laboratory
T-12
Mailstop B268
Los Alamos, NM 87545

Dr. Thomas Zacharia
Oak Ridge National Laboratory
Bldg 4508
MS 6096
Oak Ridge, TN 37831-6096

Prof. Rudy Wenk
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Karl-Heinz Winkler
Los Alamos National Laboratory
C-DO
Mailstop B260
Los Alamos, NM 87545

Dr. George Yoder
ONR Code 1131
800 N. Quincy St.
Arlington, VA 22217-5000

Pascal Yvon
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Forum on Ion Beam Analysis
Thursday, August 8, 1991

Session I

Chairman: J. Tesmer

- 8:45 – 9:00 *Welcome — Don Parkin, Center for Materials Science, Los Alamos National Laboratory*
- 9:00 – 9:45 *Energy Loss — Eero Rauhala, University of Helsinki, Finland*
(Monitors: M. Bozoian and J. Debrun)
- 9:45 – 10:00 Discussion
- 10:00 – 10:30 Break
- 10:30 – 11:15 *Nuclear Reaction Theory — Michael Bozoian, Los Alamos National Laboratory* (Monitors: E. Rauhala and J. Tesmer)
- 11:15 – 11:30 Discussion
- 11:30 – 12:15 *Backscattering Analysis — John Leavitt, University of Arizona; Martha Weller, Middle Tennessee State University*
(Monitors: J. Mayer and W. Lanford)
- 12:15 – 12:30 Discussion
- 12:30 – 2:00 Lunch

Session II

Chairman: M. Nastasi

- 2:00 – 2:45 *Elastic Recoil Detection — J. Charles Barbour, Sandia National Laboratories* (Monitors: M. Weller and M. Swanson)
- 2:45 – 3:00 Discussion
- 3:00 – 3:45 *Nuclear Reaction Analysis — Juha-Pekka Hirvonen, Technical Research Centre of Finland* (Monitors: M. Nastasi and J. Davies)
- 3:45 – 4:00 Discussion
- 4:00 – 4:30 Break
- 4:30 – 5:15 *Nuclear Reactions for Hydrogen Analysis — William Lanford, SUNY at Albany* (Monitors: J. Barbour and R. Weller)
- 5:15 – 5:30 Discussion
- 5:30 – 6:30 Reception at the Study Center

Forum on Ion Beam Analysis

Friday, August 9, 1991

Session III

Chairman: J. C. Barbour

- 8:00 – 8:45 *Channeling — Max Swanson, University of North Carolina at Chapel Hill*
(Monitors: J. Mayer and J-P. Hirvonen)
- 8:45 – 9:00 Discussion
- 9:00 – 9:45 *Instrumentation — Robert Weller, Vanderbilt University*
(Monitors: J. Leavitt and J. Davies)
- 9:45 – 10:00 Discussion
- 10:00 – 10:30 Break
- 10:30 – 11:15 *Charged Particle Activation Analysis — Jean-Luc Debrun, CNRS-CERI, France*
(Monitors: R. Weller and E. Rauhala)
- 11:15 – 11:30 Discussion
- 11:30 – 12:15 *Pitfalls In Ion Beam Analysis — John Davies, Western Ontario University*
(Monitors: M. Swanson and C. Maggiore)
- 12:15 – 12:30 Discussion
- 12:30 – 2:00 Lunch

Executive Sessions

Session IV

C. Maggiore

- 2:00 – 3:00 *Round Table Discussion of Appendices — Michael Nastasi, Los Alamos National Laboratory*
- 3:00 – 3:30 Break
- 3:30 – 4:15 *Discussion on Radiation Safety — Paul DeLuca, U. of Wisconsin*
- 4:15 – 5:00 *Monitors/Editors Working Groups*
- 6:30 Dinner

Saturday, August 10, 1991

Session V

Chairman: J. Mayer

- 8:30 – 12:00 *Chapter Assessments, Status and Summary*

Los Alamos National Laboratory
Center for Materials Science
CMS Conference Room
August 8 - 10, 1991

LIST OF PARTICIPANTS

J. Charles Barbour
Sandia National Laboratories
Div. 1111
Albuquerque, NM 87185

John A. Davies
McMaster University
Engineering Physics Dept.
ABB-448
1280 Main St. W.
HAMILTON, Ont.
CANADA L8S 4M1

A. M. Boring
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Jean-Luc M. Debrun
CNRS-CERI
3A rue de la Ferolerie
45071 Orleans
FRANCE

Michael Bozoian
Los Alamos National Laboratory
T-2
Mailstop B243
Los Alamos, NM 87545

Dr. Paul De Luca
University of Wisconsin
Department of Medical Physics
1300 University Ave. Room 1530
Madison, WI 53706

Ian H. Campbell
Los Alamos National Laboratory
MEE-11
Mailstop D429
Los Alamos, NM 87545

Anthony DiGiovanni
Los Alamos National Laboratory
MST-5
Mailstop E546
Los Alamos, NM 87545

Dr. Barney Doyle
Sandia National Laboratory
P.O. Box 5800
Division 1111
Albuquerque, NM 87185

Thomas Jervis
Los Alamos National Laboratory
DIR-ESD
Mailstop A103
Los Alamos, NM 87545

Lynn Foster
Los Alamos National Laboratory
P-10
Mailstop K764
Los Alamos, NM 87545

Pang-Jen Kung
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

Donald Cort Gautier
Los Alamos National Laboratory
MST-7
Mailstop K763
Los Alamos, NM 87545

William A. Lanford
SUNY/Albany
Physics Department
Albany, NY 12222

J. P. Hirvonen
Technical Research Centre of Finland
Laboratory of Metallurgy
P.O. Box 113
02150 Espoo
FINLAND

Bernhard Laurich
Los Alamos National Laboratory
MEE-11
Mailstop D429
Los Alamos, NM 87545

Kevin Hubbard
Los Alamos National Laboratory
MST-7
Mailstop K765
Los Alamos, NM 87545

John A. Leavitt
University of Arizona
Dept. of Physics
Tucson, AZ 85721

David S. Lieberman
Los Alamos National Laboratory
T-11
Mailstop K765
Los Alamos, NM 87545

Michael Nastasi
Los Alamos National Laboratory
MST-7
Mailstop K765
Los Alamos, NM 87545

Li Luo
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Eero J. M. Rauhala
University of Helsinki
Accelerator Lab.
Dept. of Physics
SF-00170 Helsinki
FINLAND

Carl Maggiore
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Jim Rubin
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

James W. Mayer
Cornell University
Bard Hall
Ithaca, NY 14853

David C. Smith
Los Alamos National Laboratory
INC-4
Mailstop C346
Los Alamos, NM 87545

Robert Messner
Los Alamos National Laboratory
MST-7
Mailstop K765
Los Alamos, NM 87545

James Steele
Los Alamos National Laboratory
NMT-5
Mailstop E506
Los Alamos, NM 87545

Max L. Swanson
University of North Carolina
Dept. of Physics & Astronomy
Chapel Hill, NC 27599-3255

Joe Tesmer
Los Alamos National Laboratory
P-10
Mailstop K764
Los Alamos, NM 87545

Martha R. Weller
Vanderbilt University
Box 1687
Station B
Nashville, TN 37335

Robert A. Weller
Vanderbilt University
Box 1687
Station B
Nashville, TN 37335

Pascal Yvon
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Agenda
 "Phenomenology and Applications of High Temperature Superconductors,
 The Los Alamos Symposium: 1991"
 August 22-24, 1991
 Fuller Lodge

Thursday, August 22, 1991

Registration:	8:00 - 8:30 a.m.
<u>Morning Session: Thin Films and Microwave Properties</u>	8:30 - 12:00 noon
Session Chairman: J. Robert Schrieffer	
Eugene Wewerka: Welcome	8:30 - 8:40 a.m.
Organization of the meeting:	8:40 - 8:50 a.m.
Shoji Tanaka: Keynote Address	8:50 - 9:30 a.m.
Aharon Kapitulnik: Thin Films and Multilayer HTS*	9:30 - 10:30 a.m.
Coffee Break:	10:30 - 11:00 a.m.
George Grüner: Microwave Properties*	11:00 - 12:00 noon
Poster Announcements:	12:00 - 12:30 p.m.
Lunch:	12:30 - 1:30 p.m.
Poster Session Chairman: Masahiko Inui	
Poster Session:	1:30 - 2:30 p.m.
<u>Afternoon Session: Textured Materials and Josephson Junctions</u>	2:30 - 5:50 p.m.
Session Chairman: Seb Doniach	
Masato Murakami: Textured Materials*	2:30 - 3:30 p.m.
Coffee Break:	3:30 - 3:50 p.m.
John Clarke: Josephson Junctions*	3:50 - 4:50 p.m.
Douglas Finnemore: Critical Fields etc.*	4:50 - 5:50 p.m.
<u>Thursday Evening:</u>	
Director's Hosted Reception: University House	6:00 - 7:00 p.m.
Dinner at Katherine's:	7:30 - 10:00 p.m.

Friday, August 23, 1991

<u>Morning Session:</u> <u>Vortex Lattice Structure and Melting</u>	8:30 - 12:00 noon
Session Chairman: Larry Campbell	
David Nelson: Correlations and Transport in Vortex Liquids	8:30 - 9:30 a.m.
Peter Gammel: Experimental Properties of Vortex Glass Phase*	9:30 - 10:30 a.m.
Coffee Break:	10:30 - 11:00 a.m.
Daniel Fisher: Phase Transitions and Transport in Anisotropic Superconductors with Large Thermal Fluctuations	11:00 - 12:00 p.m.
Poster Announcements:	12:00 - 12:30 p.m.
Lunch:	12:30 - 1:30 p.m.
Poster Session Chairman: Masahiko Inui	
Poster Session:	1:30 - 2:30 p.m.
<u>Afternoon Session:</u> <u>Vortex Pinning and Creep</u>	2:30 - 6:00 p.m.
Session Chairman: Marty Maley	
Gabe Aeppli: Neutron Scattering*	2:30 - 3:30 p.m.
Coffee Break	3:30 - 4:00 p.m.
Boris Ivlev: Resistance, Flux Motion and Pinning in High Temperature Superconductors	4:00 - 5:00 p.m.
Peter Kes: Vortex Pinning and Creep Experiment	5:00 - 6:00 p.m.
Friday Evening:	
Dinner at DeColores:	7:30 - 10:00 p.m.

Saturday, August 24, 1991

Morning Session: Survey of Applications and Summary
Session Chairman: Jim Smith

8:30 - 12:00 noon

Robert Hammond: Survey of Electronics Applications*

8:30 - 9:30 a.m.

David Larbalestier: Survey of Applications, High Current*

9:30 - 10:30 a.m.

Coffee Break:

10:30 - 11:00 a.m.

Michael Tinkham: Summary

11:00 - 12:00 noon

*Some titles are tentative.

PHENOMENOLOGY AND APPLICATIONS OF HIGH
TEMPERATURE SUPERCONDUCTORS:
THE LOS ALAMOS SYMPOSIUM - 1991

Center for Materials Science
and
Exploratory Research Development Center
Los Alamos National Laboratory
August 22 - 24, 1991

Elihu Abrahams
Rutgers University
Physics & Astronomy Department
Piscataway, NJ 08855

Alan R. Bishop
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

Gabriel Aeppli
AT&T Bell Laboratories
600 Mountain Avenue
Murray Hill, NJ 07974-2070

A. M. Boring
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Al J. Arko
Los Alamos National Laboratory
P-10
Mailstop K764
Los Alamos, NM 87545

Laurence J. Campbell
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

Kevin Bedell
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

John Clarke
University of California
Department of Physics
Berkeley, CA 94720

Dermot Coffey
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Sebastian Doniach
Stanford University
Applied Physics
Stanford, CA 94305-4090

Bryan R. Coles
Imperial College of Sciences
& Technology
Prince Consort Rd.
London SW7 2B2
UNITED KINGDOM

Douglas K. Finnemore
Iowa State University
Department of Physics
Ames, IA 50011

Nicholas Coppa
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

Daniel S. Fisher
Harvard University
Lyman Lab.
Department of Physics
Cambridge, MA 02138

George W. Crabtree
Argonne National Laboratory
MSD 223
Argonne, IL 60439

Zachary Fisk
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Luke L. Daemen
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

Peter L. Gammel
AT&T Bell Laboratories
600 Mountain Avenue
Room 1D221
Murray Hill, NJ 07974

Allen M. Goldman
University of Minnesota
Physics Department
Minneapolis, MN 55455

Marilyn E. Hawley
Los Alamos National Laboratory
MST-7
Mailstop K762
Los Alamos, NM 87545

Kenneth E. Gray
Argonne National Laboratory
Bldg - 223
Argonne, IL 60439

Masahiko Inui
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

George Gruner
University of California, Los Angeles
Department of Physics
405 Hilgard Ave.
Los Angeles, CA 90024-1547

Boris Ivlev
University of Southern California
Department of Physics
Los Angeles, CA 90089-0484

P. Chris Hammel
Los Alamos National Laboratory
P-10
Mailstop K764
Los Alamos, NM 87545

Aharon Kapitulnik
Stanford University
Department of Applied Physics
Stanford, CA 94305-4085

Robert Hammond
Superconductors Technologies Inc.
460 Ward Dr.
Suite 7
Santa Barbara, CA 93111

Peter H. Kes
Kamerlingh Onnes Laboratory
P.O. Box 9506
2300 RA Leiden
THE NETHERLANDS

Vladimir G. Kogan
Ames Laboratory
Physics Department
Ames, IA 50011

Martin P. Maley
Los Alamos National Laboratory
ERDC
Mailstop K764
Los Alamos, NM 87545

Pang-Jen Kung
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

Alexis P. Malozemoff
American Superconductor
149 Grove St.
Watertown, MA 02172

David C. Larbalestier
University of Wisconsin-Madison
College of Engineering
1500 Johnson Drive
Madison, WI 53706

Michael McHenry
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

Ross Lemons
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

David Meltzer
University of Florida
Quatum Theory Project
Williamson Hall
Gainesville, FL 32611

Li Luo
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Fred M. Mueller
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Ross E. Muenchausen
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

Dean E. Peterson
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

Masato Murakami
International Superconductivity
Tech Center
Superconductivity Research Lab.
10-13, Shinonome, 1-Chome, Koto-ku
Tokyo 135, JAPAN

David Pines
University of Illinois
1110 West Green Street
Urbana, IL 61801

David Nelson
Harvard University
Department of Physics
Cambridge, MA 02138

David W. Reagor
Los Alamos National Laboratory
MEE-11
Mailstop D429
Los Alamos, NM 87545

Thomas T. M. Palstra
AT&T Bell Laboratories
Room 1B118
600 Mountain Avenue
Murray Hill, NJ 07974

T. Maurice Rice
ETH-Honggerberg
Theoretische Physik
8093 Zurich
SWITZERLAND

Don M. Parkin
Los Alamos National Laboratory
CMS
Mailstop K765
Los Alamos, NM 87545

Douglas Scalapino
Univ. of California, Santa Barbara
Department of Physics
Santa Barbara, CA 93106

J. Robert Schrieffer
Univ. of California, Santa Barbara
Department of Physics
Santa Barbara, CA 93106

Joe D. Thompson
Los Alamos National Laboratory
P-10
Mailstop K764
Los Alamos, NM 87545

Richard N. Silver
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

Michael Tinkham
Harvard University
Physics Department
Cambridge, MA 02128

James L. Smith
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

Stuart A. Trugman
Los Alamos National Laboratory
T-11
Mailstop B262
Los Alamos, NM 87545

Kendall Springer
Los Alamos National Laboratory
MEE-11
Mailstop D429
Los Alamos, NM 87545

Valeri Vinokur
Argonne National Laboratory
MSD
9700 South Cass Avenue
Argonne, IL 60439

Shoji Tanaka
International Superconductivity
Tech Center
Superconductivity Research Lab
10-13 Shinonome, 1-Chome
Koto-ku, Tokyo 135
JAPAN

Eugene Wewerka
Los Alamos National Laboratory
ADCM
Mailstop A102
Los Alamos, NM 87545

John Wilkins
Ohio State University
Department of Physics
4100 Smith Lab.
174 West 18th Ave.
Columbus, OH 43210

Stuart A. Wolf
Head, Materials Physics Branch
Code 6340
Naval Research Laboratory
Washington, DC 20375-5000

Xindi Wu
Los Alamos National Laboratory
ERDC
Mailstop K763
Los Alamos, NM 87545

NATIONAL HIGH MAGNETIC FIELD LABORATORY
WORKSHOP ON LONG PULSE MAGNETS

University House Los Alamos National Laboratory
Dwight G. Rickel, Chairman

Agenda

September 30, 1991 (Monday)

- 8:30 a.m. Overview of NHMFL, Pulsed Magnet Program
Don Parkin, Director, CMS
- 9:00 a.m. Design Parameters and Status of NHMFL Pulsed Magnet Development Project
60-T System, Jim Sims, LANL
50-T System, John Rogers, LANL
- 9:30 a.m. Overview of Design and Status of 60-T Long Pulse Magnet Program at the
University of Amsterdam
Paul Frings, University of Amsterdam
- 10:00 a.m. Design Parameters and Performance of Composite Coils
Luc Van Bockstal, Catholic University-Leuven
- 10:30 a.m. Break
- 10:45 a.m. Overview and Status of Princeton University Long Pulse Magnet Program
Peter Bonanos, Princeton University
- 11:15 a.m. Status and Development of Pulsed Power Systems in Support of the NHMFL
Pulsed Magnet Program
Heinrich Boenig, LANL
- 11:45 a.m. Break for Lunch
- 1:00 p.m. Status of Materials Development in Support of Pulsed Magnet Program
Mary Ann Hill, LANL
- 2:00 p.m. General Discussion and Establishment of Collaborative Programs

Conductors and Insulating Systems
Jim Sims, Chairperson

5:15-6:15 p.m. — Cocktail Reception at the University House

Agenda — Continued

October 1, 1991 (Tuesday)

- 8:30 a.m. Continuation of Discussions —
Long Pulse Magnet Design and Fabrication
Dwight Rickel, Chairperson
- 10:30 a.m. Break
- 10:45 a.m. Resume Discussions
- 11:45 a.m. Break for Lunch
- 1:00 p.m. Formulation of Collaborative Agreements
- 2:30 p.m. Break
- 2:45 p.m. Draft Report of Workshop
- 5:00 p.m. Adjournment

Objectives of Workshop

Organization of Materials Development and Selection Efforts. The workshop should work toward the establishment of cooperative programs focused establishing areas of concern for materials development. The efforts should be focused at microcomposites, e.g., Cu-Nb, Cu-Ag, Cu-Be, and other systems, and macrocomposites/filamentary re-inforced systems of potential use to magnet development. Mechanisms to share data and the establishment of a "Clearing House" to create a database that is made available to all participants should be considered.

Establishment of Essential Features of Cooperative Programs. There has been tentative agreement to establish cooperative programs focused at the development of pulsed magnet systems. These informal agreements have been between the NHMFL, Princeton University, University of Amsterdam, Catholic University-Leuven, and the European 100-T Wire Project. The participants cannot negotiate the final agreements because such action will require input and approval from those not participating, but the workshop should draft proposals that will lead to a formal agreement between participating institutions.

Identification of Development Areas With Designated Institutional Responsibility. A division of areas of responsibility should be established so that project goals are met in a cost-effective and timely fashion. There may be planned duplication of efforts in critical areas or addressing design and development issues that are power-system specific. A schedule for future meetings with goals should be discussed and established.

Long pulse magnet discussion

ISSUES

1. Number of coils
2. conductor aspect ratio and size
3. winding configurations
 - a. continuous single winding
 - b. adjacent parallel turns
 - c. parallel layers
 - d. pancake
4. insulation methods
 - a. inner layer insulation
 - b. wire insulation
5. reinforcement methods
 - a. outer thick wall container
 - b. fiber belts
 - c. fiber on wires
 - d. end walls
 - e. hydrostatic requirements for coil volume
6. cooling requirements
 - a. conduction from outer coil surfaces
 - b. any other options?
7. Winding systems
 - a. should we develop an in house capability
 - b. can a vendor satisfy our needs?
8. coil lifetime
 - a. number of shots per day
9. testing program for coil design
 - a. can we build scaled prototypes?
 - b. can we use capacitive system to do testing?
10. computer modeling
 - a. What tools are available?
 - b. can good modelling insure success?

NATIONAL HIGH MAGNETIC FIELD LABORATORY
WORKSHOP ON LONG PULSE MAGNETS

September 30th and October 1st 1991

ATTENDANCE LIST

NAME	ADDRESS, TELEPHONE
Luc Van Bockstal	Laboratory for Low Temperatures and High Field Physics K. V. Leuven Celestýhen Laah 200D B-3001 Heverlee Belgium Tel (32)16-201015 FAX (32)16-201368
Heinrich Boenig	Los Alamos National Laboratory M6 M.S. E536 Los Alamos, NM 87545 Tel 505 667 4404 FAX 505 665 4311
Peter Bonanos	Princeton University Plasma Physics Laboratory P.O. Box 451 Princeton, NJ 08543 USA Tel 609-243-3201 FAX 609-243-2111
Bruce Freemam	Los Alamos National Laboratory M6 M.S. J970 Los Alamos, NM 87545 USA Tel 505-667-6539 FAX 505-665-3050
Franz Frieibert.	Florida State University Keen Building, B159 Tallahassee, FL 32306 USA Tel 904-644-5075
C. M. Fowler	Los Alamos National Laboratory M6 M.S. J970 Los Alamos NM 87545 Tel 505-667-6525 FAX 505-665-3050

Paul Frings

Van der Waals-Zeeman Lab.
University of Amsterdam,
Valckernierstraat 65
1018 xe Amsterdam
The Netherlands

Tel 31-20-5255744
5663
FAX 31-20-5255788

Mary-Ann Hill

Los Alamos National Laboratory
MST-7 M.S. G770
Los Alamos, NM 87545
Tel 505 665 3658

Marion Hodgdon

Los Alamos National Laboratory
M6 M.S. E536
Los Alamos, NM 87545
Tel 505 665 6504
FAX 505 665 4311

Bob Langer

Los Alamos National Laboratory
M6 M.S. E536
Los Alamos, NM 87545
Tel 505 665 6504
FAX 505 665 4311

Stephen Lloyd

Los Alamos National Laboratory
M4 M.S. P940
Los Alamos, NM 87545
Tel 505 665 2744

Emmanuel Lopez

Los Alamos National Laboratory
M-6 M.S. E536
Los Alamos, NM 87545
Tel 505 665 4014
FAX 505 665 4311

Henn Oona

Los Alamos National Laboratory
M-6 MS J970
Los Alamos, NM 87545
Tel 505 667 0749
FAX 505 665 3050

Don Parkin

Los Alamos National Laboratory
CMS M.S. K765
Los Alamos, NM 87545
USA Tel 505 667 8455
FAX 505 665 2992

Dwight Rickel

Los Alamos National Laboratory
M6 M.S. J970
Los Alamos, NM 87545
USA Tel 505 667 1222
or 6881
FAX 505 665 3050

John Rogers

Los Alamos National Laboratory
M6 M.S. E536
Los Alamos, NM 87545
Tel 505-667 5427
FAX 505-665 4311

Hans J. Schneider-Muntau

NHMFL
Florida State University
Tallahassee, FL 32306
USA Tel

Jim Sims

Los Alamos National Laboratory
M6 MS E536
Los Alamos, NM 87545
USA Tel 505 665 1975
FAX 505 665 4311

APPENDIX D

CMS PERONNEL
AND
ASSOCIATES

APPENDIX D

Center for Materials Science

TA-3, SM-32, MS K765, 667-9243

Parkin, Don M.; Center Director	7-8455
Boring, A. M.; Deputy Director	7-9245
Clogston, Albert M.	7-0963
Fisk, Zachary	5-0892
Kocks, U. Fred	7-9323
Maggiore, Carl J.	7-6133
Mitchell, Terence E.	7-0938
Mueller, Fred M.	7-9244
Schwarz, Ricardo B.	7-8454
Gibala, Ron; Bernd Matthias Scholar	5-1320
Sham, Lu; Bernd Matthias Scholar	
Wenk, Rudy; Bernd Matthias Scholar	7-6337
McCulla, Bettye; Admin. Asst.	7-9243
Lauer, Laurie; Admin, Asst.	7-3213
Romero, Brenda; Wordprocessor	7-0970
Hollander, Mark; Technician	7-4377
Nye, Donald; Technician	7-6713
Smith, James F.; Technician	7-9585
Trickey, Samuel, LTVSM	
Chen, Shuhrong; Postdoc	5-0982
Coffey, Dermot; Postdoc	7-9556
Daemen, Luc; Postdoc	5-0419
Eriksson, Olof; Postdoc	5-4005
Inui, Masahiko; Postdoc	7-9860
Koike, Jun; Postdoc	5-4006
Luo, Li; Postdoc	5-4003
Srinivasan, Sreeram; Postdoc	5-1171
Suematsu, Hisayuki; Postdoc	5-4002
Leisure, Robert; Collaborator	7-6337
Brandow, Baird, Guest Scientist	5-1160
Bennett, Kristin; GRA	
Burke, Tim; GRA	
Desch, Paul; GRA	
Heidelberg, Florian; GRA	
McClellan, Ken; GRA	
Poole, Warren; GRA	
Rubin, James; GRA	
Unal, Ozer; GRA	
Yvon, Pascal; GRA	
Dick, Aaron; UGS	
Ortiz, Melissa; UGS	

Affiliates

Arko, A., P-10	5-0758	MS K764
Albers, R. C., T-11	5-0417	MS B262
Basu, Soumendra, MST-7	5-4003	MS K765
Bedell, K., T-11	5-1314	MS K765
Beery, J., MEE-11	7-1499	MS D429
Beyermann, W., P-10	5-0634	MS K764
Bishop, A. R., T-11	7-6491	MS B262
Blasic, J., EES-3	7-6815	MS C335
Canfield, P., P-10	7-4838	MS K764
Conradson, Steve, INC-4	7-1001	MS C354
Cox, L. E., NMT-5	7-2346	MS E506
Dye, R., CLS-2	5-4002	MS K763
Evans, C., P-10	7-4377	MS K764
Fowler, C. M., M-6	7-6525	MS J970
Freeman, B. L., M-6	7-6539	MS J970
Hammel, P. C., P-10	5-0759	MS K764
Hawley, Marilyn, MST-7	5-4091	MS K762
Heffner, R., P-10	7-4838	MS K764
Hill, Mary Ann, MST-6	5-3658	MS G770
Hirvonen, J-P., MST-7	5-1313	MS K765
Hubbard, K. M., MST-7	5-4004	MS K765
Hults, W. L., ERDC	7-4476	MS K763
Hundley, M. F., P-10	7-4129	MS K764
Jervis, T. R., MST-7	7-1531	MS E549
King, J. C., M-6	5-0348	MS J970
Laurich, B. K., MEE-11	5-0333	MS D429
Leisure, R., P-10	7-6337	MS K765
Lomdahl, P., T-11	5-0461	MS B262
Lu, C.S., T-11	5-2489	MS B262
Martin, J., CLS-2	5-1138	MS K765
McDowell, H. K., CLS-2	7-4686	MS G738
Migliori, Albert, P-10	7-2515	MS K764
Muenchausen, R. E., ERDC	7-1753	MS K763
Mustre de Leon, J., MEE-11	5-4008	MS G429
Nastasi, Mike, MST-7	7-7007	MS K765
Petrovic, J. J., MST-4	7-0125	MS G771
Raistrick, Ian D., MEE-11	7-9741	MS D429
Rollett, Tony, MST-6	5-0982	MS K765
Robertson, E., MST-6	7-2465	MS G770
Salazar, K., ERDC	5-1762	MS K763
Schofield, T., MST-6	5-2364	MS K765
Sickafus, K., MST-4	5-3457	MS K762
Sizek, H., MST-5	7-6967	MS G730
Smith, J. L., ERDC	7-4476	MS K763
Stout, M. G., MST-5	7-6750	MS G730
Swanson, Basil, INC-4	7-6045	MS C346
Takigawa, M., P-10	5-0189	MS K764
Tesmer, J., P-10	7-6370	MS K765
Thompson, J. D., P-10	7-6416	MS K764
Zocco, T. G., MST-5	7-4481	MS G730
Ward, J. W., NMT-5	7-2349	MS E506
Ward, W., P-10	7-5150	MS K764
Wills, J., T-1	5-2308	MS B221

Collaborators

Philip B. Allen, State University of New York at Stony Brook
 Michael Aziz, Harvard University
 Alexander Balatsky, University of Illinois
 Soumendra Nath Basu, Boston University
 Ward P. Beyermann, University of California, Riverside
 Gilbert Blondiaux, Centre Nationale de la Recherche Scientifique, Orleans, France
 Raul Bolmaro, Universidad Nacional de Rosario, Argentina
 Richard Brook, University of Leeds, Leeds, England
 Gilles R. Canova, Laboratoires de Physique Et Mec, Metz, France
 Niels E. Christensen, Max-Planck Inst. fur Festforperforschung, Stuttgart, West Germany
 Andrew P. Clark, Utah State University
 Bryan Coles, Imperial College, London, England
 Alfred R. Cooper, Case Western Reserve University
 Bernard R. Cooper, University of West Virginia
 Jack E. Crow, Florida State University
 Abhaya Krishna Datye, University of New Mexico
 Paul Dawson, Cornell University
 Jean L. Debrun, Centre Nationale de la Recherche Scientifique, Orleans, France
 Roger D. Doherty, Drexel University
 Kenneth Easterling, Lulea University, Lulea, Sweden
 Charles M. Falco, University of Arizona
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 Karen L. Kavanagh, University of California, San Diego
 Vladimir Kogan, Ames Laboratory
 Veli-Tapani Kuokkala, Tampere University of Technology, Finland
 Jon M. Lawrence, University of California, Irvine
 Robert Leisure, Colorado State University
 M. Brian Maple, University of California, San Diego
 James W. Mayer, Cornell University
 Heinz Mecking, University Hamburg-Hamburg, Hamburg, West Germany
 Carlos Melo, Stanford University
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 Hartmut Monien, University of Illinois
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 Philip G. Nash, Illinois Institute of Technology
 Tayfur Ozturk, Middle East Technical University, Turkey
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 Christopher Pethick, University of Illinois
 Khandker F. Quader, Rutgers University
 Dierk Rainer, Universitat Bayreuth, West Germany
 Peter Riseborough, Polytechnic Institute of New York
 Seven Anders Rosengren, University of Uppsala, Sweden
 Francois Rossi, CEA Valduc, Paris, France
 Andrei Ruckenstein, University of California, San Diego
 Pekka R. Ruuskanen, Tampere University, Tampere, Finland
 Hiroshi Sato, Purdue University\

Collaborators cont.

Cheng Saw, Hoechst Celanese Research Co.
Gerhard H. Schadler, ETH-Honggerberg, Zurich, Switzerland
Joseph Serene, Naval Research Laboratory
Boris Shapiro, Isreal Institute of Technology, Israel
Michael Springborg, Nordita, Copenhagen, Denmark
Naresh N. Thadhani, New Mexico Institute of Mining and Technology
Tuomo Tiainen, Tampere University, Tampere, Finland
Carlos Tome, University Nacionale de Rosario, Rosario, Argentina
Ozer Unal, Case Western Reserve University
Victor Van Doren, University of Antwerp, Antwerp, Belgium
Vaclav Vitek, Technical University, Vienna, Austria
Luc Van Bockstal, Katholieke Universiteit Leuven, Belgium
P. Weinberger, Technical University of Vienna, Austria
H.-Rudy Wenk, University of California, Berkeley
Clare Yu, University of California, Irvine

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John S. Faulkner, Florida Atlantic University
 Arthur J. Freeman, Northwestern University
 Borje Johansson, University of Uppsala, Sweden
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 Douglas Scalapino, University of California, Santa Barbara
 Lu Sham, University of California, San Diego
 John Wilkins, Ohio State University
 Dieter Wohlleben, University of Kln, Kln, West Germany
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