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***Edited by
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Institute of Geophysics and Planetary Physics
University of California***

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Section I. Overview

The Institute of Geophysics and Planetary Physics (IGPP) is a Multicampus Research Unit of the University of California. The IGPP was founded in 1946 at UC Los Angeles to further research in the earth and planetary sciences and in related fields.

The Institute now has branches at UC Los Angeles, UC San Diego, and UC Riverside, and at the Los Alamos and Lawrence Livermore National Laboratories.

The University-wide IGPP has played an important role in establishing interdisciplinary research in the earth and planetary sciences. For example, the IGPP was instrumental in founding the fields of physical oceanography and space physics, disciplines that had fallen "between the cracks" of university departments. Because of its multicampus orientation, the IGPP has sponsored inter-institutional consortia in the earth and planetary sciences. Each of the five branches has a different intellectual emphasis because of the interplay between strengths of the campus departments and the national laboratories.

Livermore IGPP (IGPP-LLNL), the youngest of the five branches, was approved by the Regents of the University of California in 1982. It emphasizes research in seismology, geochemistry, cosmochemistry, high-pressure sciences, and astrophysics. IGPP-LLNL provides a venue for studies of the basic aspects of these fields, complementing LLNL programs that pursue applications of these disciplines in national security and energy research. IGPP-LLNL is directed by Claire Max and is structured around three Research Centers. The Center for Geosciences, headed by George Zandt and Frederick Ryerson, focuses on research in geophysics and geochemistry. The Center for High-Pressure Sciences, headed by William Nellis, sponsors research on the properties of planetary materials and on the synthesis and preparation of new materials using high-pressure processing. The Astrophysics Research Center, headed by Charles Alcock, provides a home for theoretical and observational astrophysics. It provides an interface with the Physics Department's Laboratory for Experimental Astrophysics and with other astrophysics efforts at LLNL.

Since January 1987, the IGPP-LLNL and the IGPP University-wide administration have taken on administrative responsibility for the UC Accelerator Mass Spectrometry (AMS) Facility, one of 19 beamlines at LLNL's new multipurpose accelerator laboratory. Research by UC users at this facility is multidisciplinary, with applications in paleoclimatology, paleontology, archaeology, cosmochemistry, global warming, pollutant tracking, oceanography, and biomedical sciences. The LLNL Center for Accelerator Mass Spectrometry, directed by Jay Davis, oversees operations and scientific collaborations of the UC AMS Facility.

Like the IGPP branch at Los Alamos, IGPP-LLNL facilitates scientific collaborations between UC researchers and those at the national laboratories in areas related to earth and planetary sciences. It sponsors the University Collaborative Research Program (UCRP), which provides funds to UC scientists for joint research projects with LLNL. Two goals of UCRP are to enrich research opportunities for

UC scientists by making available LLNL's facilities and expertise and to broaden the scientific program at LLNL through collaborative or interdisciplinary work with UC researchers. UCRP funds (provided jointly by the Regents of the University of California and by the Director of LLNL) are awarded annually* on the basis of brief proposals, which are reviewed by a committee of scientists from UC campuses, LLNL programs, external universities, and research organizations. Typical funding for a collaborative research project ranges from \$5,000 to \$25,000 per year. Funds are used for a variety of purposes, including support for visiting graduate students, postdoctoral fellows, faculty, experimental facility costs, released-time salaries for LLNL scientists, and supercomputing time.

Although LLNL staff assigned to IGPP is relatively small (presently about five full-time equivalents), IGPP's Research Centers have become lively research organizations since 1984. The activity is possible because of IGPP support for a substantial group of resident postdoctoral fellows, because of the 30 or more UCRP collaborative projects funded each year, and because IGPP hosts a variety of visitors, guests, and faculty members (from UC and other institutions) on sabbatical leave. To focus attention on areas of current interest in the geosciences and astrophysics, IGPP-LLNL hosts conferences and workshops. Most recently, IGPP and UC-Santa Cruz cosponsored the 84th Annual Meeting of the Seismological Society of America. IGPP-LLNL also organizes three seminar series: one in astrophysics, one in high-pressure sciences, and one in the earth sciences. Section IV of this report lists the 1990 seminars.

Figure 1.
Geographical distribution of (a) total funds awarded and (b) number of awards to each UC campus under the IGPP-LLNL University Collaborative Research Program in FY 90. Northern UC campuses received 58% of funds awarded and 62% of total number of awards. UC campuses received a total of \$532,800 and 29 awards.

* For information about the University Collaborative Research Program, including guidelines for submitting proposals, contact Christina Budwine, Operations Manager, IGPP-LLNL, L-413, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94550. Tel. (415) 423-4476. E-mail address: budwine@sunlight.llnl.gov

Figures 1 to 4 give a statistical overview of IGPP-LLNL's University Collaborative Research Program (informally called the "mini-grant" program). Figure 1 shows the distribution of UCRP awards to UC campuses. More than half of the UCRP projects in FY 90 involved campuses in Northern California (Berkeley, Santa Cruz, and Davis). Since the Livermore site is less than a two-hour drive from each of these campuses, this result should not be surprising. Convenient airplane connections to the Los Angeles and San Diego areas help keep participation from Southern California campuses high (nearly 42% in FY 90).

Figure 2 shows the funds requested and awarded under UCRP in FY 90, distributed among the three IGPP-LLNL Research Centers. Investigators in the geosciences requested and received the largest funding. Geosciences was the most competitive area, as measured by the ratio of funds awarded to funds requested. The UCRP program at LLNL awarded about half of the total funds requested in FY 90.

Figure 3 shows the superconductor time requested by and awarded to the three Research Centers. High-Pressure Sciences received the most time in FY 90.

Beginning in FY 87, IGPP-LLNL has maintained a bibliography of published research papers resulting from UCRP collaborative projects and from research by

Figure 2. Funds requested and awarded to Research Centers under the IGPP-LLNL University Collaborative Research Program in FY 90. Geosciences attracted the largest number of proposals and received the most funds in FY 90.

Figure 3. Supercomputer time requested and awarded to Research Centers under the IGPP-LLNL University Collaborative Research Program in FY 90. High-Pressure Sciences received the most superconductor time in FY 90. Cray awards to all UC campuses totaled 195 hours.

the IGPP's staff, postdoctoral fellows, and consultants. Section V of this report lists papers published in 1990, and (for 1989 and 1988) adds papers not listed in the 1989 IGPP Annual Report. The research productivity is impressive: over 400 IGPP-LLNL publications have appeared since 1984 and another 40 are in press. Figure 4 shows the growth of IGPP-LLNL publications since 1987. The abundance of publications from IGPP collaborative projects is a measure of the significance of the results obtained in these projects. Table 1 shows the number of UC faculty, staff, and students involved in UCRP projects in FY 90.

Figure 4. Number of IGPP-LLNL papers published in refereed journals and conference proceedings, by fiscal year. Institute participants publish 90 to 100 papers a year.

Table 1. UC faculty, staff, and students involved in UCRP projects in FY 90. A total of 42 LLNL scientists collaborated in this work.

Campus	Faculty	Staff	Students
UCB	7	5	8
UCD	3	1	6
UCLA	5	1	5
UCR	1	0	1
UCSB	1	0	1
UCSC	2	5	5
UCSD	3	2	3
Other scholars	2	1	0
Total	24	15	29

Section II. Highlights of the 1990 Fiscal Year

Center for High-Pressure Sciences

The purpose of the Center for High-Pressure Sciences is to make LLNL's high-pressure experimental facilities and modeling capabilities available for collaborations between UC researchers and LLNL scientists. The collaborations include the use of experimental facilities at LLNL, joint theoretical work, use of LLNL supercomputers for theoretical calculations and data analysis, and experimental work carried out at UC campuses on specimens processed at high pressures at LLNL. UC faculty members, graduate students, and postdoctoral researchers participate in the program.

Our expertise in experimental, theoretical, and computational aspects of high-pressure research encompasses geophysics, planetary physics, condensed-matter physics, chemistry, materials science, and engineering. Principal facilities and capabilities at LLNL are the following:

- *Two-stage light-gas guns*, which can be used to measure equations of state, shock-wave profiles, electrical conductivities, and emission, Raman, and absorption spectra of minerals, liquids, and metals shocked to 100 GPa (1 Mbar) dynamic pressures and to several thousand kelvins. These gas guns can also be used to synthesize new materials by application of high dynamic pressure and temperature. (Contact: Neil Holmes, 415-422-7213, and William Nellis, 415-422-7200.)
- *Diamond anvil cells* to measure equations of state by x-ray diffraction, Raman spectroscopy, and laser heating. (Contacts: Jagan Akella, 415/422-7097, and Choong-Shik Yoo, 415-422-5848.)
- *High-pressure systems* to determine stress-strain behavior, ultrasonic velocities, permeability, phase equilibria, fracture-flow properties, diffusion kinetics, and electrical and optical properties of minerals and ceramics up to 25 GPa and 2500°C. (Contact: Alfred Duba, 415-422-7306.)
- *Expertise in condensed-matter theory and modeling*, including electron-band theory, fluid perturbation and mixture theories, Monte Carlo and molecular-dynamics methods, and dense-plasma theory. (Contacts: Andrew McMahan, 415-422-7198, and Marvin Ross, 415-422-7353.)
- *Computational simulations* of the performance of gas guns and static high-pressure apparatus and of material response to dynamic loading. (Contact: Lew Glenn, 415-422-7239.)

LLNL researchers in high-pressure sciences are located in H Division (the Condensed Matter Physics Division of the Physics Department) and in the Earth Sciences Department. Shock-compression and theoretical condensed-matter research is performed in H Division. Static-pressure research and computational simulations of high-pressure phenomena are performed in the Earth Sciences Department.

Many of the Laboratory's high-pressure experimental facilities offer unique research opportunities. For example, the multianvil press and the two-stage guns are complementary facilities for synthesizing and studying geological, ceramic, and super-hard materials. The multianvil press can subject specimens with volumes of up to a cubic millimeter to pressures up to 25 GPa, temperatures up to 2500 K, and quench rates up to 100 K/s. The two-stage gun can achieve comparable and higher pressures and temperatures and can achieve quench rates more than 10^6 times greater. Thus, this pair of systems can synthesize a variety of high-pressure phases with a broad spectrum of microstructures.

Research Highlights

New Two-Stage Light-Gas Gun Facility

Our new two-stage gas-gun system has been moved to Bldg. 212, where it is now accessible to UC and other researchers without the need for a security clearance. In addition to the gun and control rooms, specimen-preparation and optical-diagnostic laboratories have also been constructed. Specimen materials and holders can be fabricated and inspected with a laser ruler, microbalance, scanning electron microscope, and vapor plater. In the diagnostic room, fast optical detection systems will be assembled and coupled to the target chamber of the gas-gun by fiber optics. The gun is 6.5 m long and can launch a 20-mm-diameter projectile to 4 km/s. A 35-mm-bore launch tube has been received for larger specimens; maximum specimen velocity in this tube is about 3 km/s.

The gun is used now for shock processing and synthesis of materials at high shock pressures. David Erskine is the technical supervisor of the facility, and Neal Hinsey is the gun operator.

Phase Transformations

Shock compression induces phase transformations at high pressures and temperatures. In FY 90, David Erskine and William Nellis performed measurements of shock-wave time histories in graphite as it transformed into diamond, thus demonstrating unambiguously that the transformation occurs by the martensitic mechanism.¹ A martensitic transformation is one in which the atoms move collectively and quickly by short displacements that take one crystal structure into another. Shock-compression of graphite (oriented along the *c*-axis of its hexagonal crystal structure) shows that the specimen transforms to diamond in about 10 ns. Although this phenomenon was predicted about 30 years ago, it had never been observed. Features that permitted observation of this prototypical high-pressure phase transformation are the high resolution of the diagnostic system and the choice of specimens. The diagnostic employed was a VISAR velocity interferometer, which uses the Doppler shift of light reflected from a shock-accelerated surface to measure the velocity history of that surface. The velocity is related simply to pressure and density.

This diagnostic tool is now available for measuring shock-induced phase transformations and longitudinal sound speeds in minerals and for diagnosing (in real time) shock synthesis of high-pressure phases.

Planetary Liquids

High shock pressures and temperatures are being used to study materials that make up the giant planets, Jupiter, Saturn, Uranus, and Neptune. The most abundant component of these planets is molecular hydrogen, and their outer envelopes are mostly H₂. It is thought that convective flow of H₂ at high pressures and temperatures within these planets contributes substantially to their external magnetic fields, especially for Jupiter and Saturn. During FY 90, the first measurement of the electrical conductivity of shock-compressed hydrogen was made by Arthur Mitchell

and William Nellis. Specimen conditions were about 20 GPa and 4000 K, which were close to conditions within the giant planets. Several more experiments are needed to determine the temperature and density dependence of the electrical conductivity and to find appropriate scaling laws for calculating the conductivity along the planetary isentropes. The experimental techniques have been developed, and the remaining conductivity data should be obtained in the coming year. These experiments are also expected to yield a measurement of the electron energy band gap for dense molecular hydrogen, which is important for testing condensed-matter physics theoretical calculations of the insulator-to-metal transition in hydrogen.

Shocked Oxides

We are continuing our study of the microstructures and properties of shocked oxides, namely quartz and high-temperature superconducting materials. The research on quartz is motivated by the need to identify the microstructures induced by the impact of meteorites; these structures can then be used to infer the shock history of minerals found in natural impact structures. This subject is timely because of current interest in determining the effects of catastrophic impacts on the history of Earth. One example is the hypothesis that a giant impact or impacts caused climatic changes that in turn caused the dinosaurs and numerous other species to become extinct. For this reason a systematic study of the microstructures of shocked quartz was performed under a UCRP grant to J. M. Christie of UC Los Angeles and William Nellis. A significant result of this work is the demonstration that optical microscopy alone is insufficient to determine whether a mineral has been shocked. For pressures below about 10 GPa, characteristic shock-induced lamellae are small enough that they can only be observed by transmission electron microscopy (TEM). Virtually all investigations of shock phenomena in minerals have heretofore used optical microscopy only.

High-temperature superconducting oxides offer prospects for developing superconducting devices cooled by liquid nitrogen. Research performed under a UCRP grant by M. B. Maple at UC San Diego and William Nellis has shown that shock-induced crystalline defects increase the critical electrical current density in grains of perovskite-type $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$. The advantageous defects are line defects—dislocations and stacking faults. These are the same type of defects found in shocked perovskite-type minerals.

Reference

1. Erskine, D. J. and Nellis, W. J., 1991, "Shock-Induced Martensitic Phase Transformation from Oriented Graphite to Diamond," *Nature* **349**, 317.

Astrophysics Research Center

The Astrophysics Research Center serves IGPP-LLNL's aims in astrophysics. This entails managing the astrophysics portion of the UCRP program and facilitating contacts between UC scientists and their LLNL counterparts. The Astrophysics Research Center also acts as the focus of astrophysics activities at LLNL by organizing the weekly astrophysics colloquium, hosting astrophysics visitors and collaborators, editing an annual Observatory Report that covers all astrophysics activities at LLNL, and performing a variety of other service functions. The staff and postdoctoral researchers in the Center carry out a significant program of astrophysics research.

The scientific staff of the Center are Charles Alcock (Astrophysics Center Head), Claire Max, and Willem van Breugel. Administrative support is provided by Christina Budwine (Operations Manager) and by secretaries Arlene Manning and JoAnne McGuire. Alan Edwards and Deanne Proctor manage the IGPP local computer network and Image Processing Facility.

Much of the research in IGPP is performed by its lively group of postdoctoral fellows. In FY 90 they were Roger Ball (previously at Cal Tech), David Bennett (Princeton), Leigh Brookshaw (Yale), Gregory Francis (MIT), Masahiro Hoshino (Goddard Space Flight Center), Eric Keto (Harvard), John Lattanzio (Canadian Institute for Theoretical Astrophysics), Robert Malaney (Cal Tech), Bradley Meyer (University of Chicago), and Marco Tavani (Columbia).

The Center (and the IGPP offices) are in LLNL Bldg. 319, which is near the offices of many LLNL astrophysicists, and is also in an area subject to minimal access control. These features make the Center ideal for the many collaborations that have developed between UC researchers and LLNL scientists.

The Astrophysics Research Center uses a variety of machines for computing. Most day-to-day work is carried out on a network of Sun workstations. Code development, image processing, and symbolic manipulation is carried out on this network. Also on the network, in addition to the main file server, are two Sun Sparcserver machines, which are dedicated to large-scale astronomical image processing; one of these machines, on loan from UC Davis, was installed at IGPP by Robert Becker of UC Davis to take advantage of the IGPP computing infrastructure. Large-scale computing is performed on a four-processor Solbourne computer (owned and operated by the LLNL Physics Department), on the Cray supercomputers in the Laboratory's Open Computing Facility, or in the National Energy Research Supercomputer Center.

Research Highlights in Astrophysics

The Astrophysics Research Center builds on the traditional strengths in astrophysics at LLNL so as to open up areas of research not previously represented at LLNL. This research ranges from small theoretical and observational projects carried out by the staff and postdoctoral fellows to large, collaborative programs involving significant involvement from outside IGPP. The following are some highlights of this research.

The MACHO Project

Charles Alcock, Timothy Axelrod, David Bennett, Kem Cook, and Hye-Sook Park have established an international collaborative program to search for "MACHOs." MACHOs (massive compact halo objects, which are like Jupiter,

only much further from us) are plausible candidates for the dark matter that makes up more than 90% of the mass of our galaxy, the Milky Way. When a MACHO moves close to the line of sight toward a star outside the Milky Way, its gravitational field acts as a lens, making the background star appear brighter. As the MACHO moves across the line of sight, the star brightens and then returns to its original brightness.

Model calculations reveal that the expected event rate, per star, is very low. For this reason, the experiment under development will involve nightly measurements of the brightnesses of millions of stars in the Magellanic Clouds, two galaxies that are "neighbors" of the Milky Way. To carry out this experiment, the LLNL team initiated a collaboration with Ken Griest, Saul Perlmutter, and Christopher Stubbs of the Center for Particle Astrophysics at UC Berkeley, and with Kenneth Freeman, Bruce Peterson, Peter Quinn, and Alexander Rodgers of the Mt. Stromlo and Siding Spring Observatories of the Australian National University. The experiment will be performed using a telescope at Mt. Stromlo, using highly innovative detectors and data processors that are under development for the project.

Discovery of the Most Distant Galaxy Known

Willem van Breugel, in collaboration with Ken Chambers and George Miley (both at Leiden Observatory, the Netherlands), has discovered the most distant galaxy known. The galaxy was found as part of an ongoing observational program to investigate the formation and evolution of radio galaxies and the origin of (radio) galaxy activity. Its redshift ($z = 3.800$) was determined from a relatively bright Lyman- α emission line and a faint carbon line using long-slit observations with the 4-m Mayall telescope at Kitt Peak National Observatory. This redshift value is supported by a strong drop in the optical continuum blueward of the Lyman- α line; such a drop would be expected either as a result of foreground absorption or a drop in the stellar continuum shortwards of Lyman α .

The origin and evolution of galaxies is one of the most challenging and rewarding studies in extragalactic astronomy because it encompasses a large variety of fundamental astrophysical disciplines, ranging from cosmology to large-scale star formation and the origin and effects of galaxy activity. The search for distant galaxies is difficult because they are rare and optically faint. Searches relying on purely optical methods have been ambiguous because many distant galaxy candidates have not revealed any detectable emission or absorption lines that would allow measurements of their redshifts. The only successful method has been to search for optical counterparts associated with extragalactic radio sources. This distant galaxy, known as 4C 41.17, is a member of a specially selected sample of radio sources with ultra-steep radio spectra and very faint optical identifications. It has been speculated for some time that such a sample might contain a large fraction of distant radio galaxies. Recent advancements in the development of sensitive optical and IR detectors enabled us to provide clear proof of the efficiency of finding distant radio galaxies using such a sample, with 4C 41.17 the current record holder.

Our observations and those of others have resulted in important discoveries, such as the elongated multimodal morphologies of high-redshift radio galaxies, the alignment of these galaxies with their associated radio sources, the correlation between ionized gas and radio source asymmetries, and the presence (at least in some cases) of polarized optical continuum. One of the most fundamental results from these observations may be that cosmology and galaxy formation studies must be concerned not only with finding distant galaxies but also with galaxy evolution and the origin and effects of early galaxy activity.

Figure 5 shows 1415 MHz and Lyman- α images of 4C 41.17 at a redshift of $z = 3.800$. Crosses show the location of prominent radio sources components. Note the alignment of the Lyman- α emission with the central two radio components, one of which (B1) contains the probable active galaxy nucleus. The optical continuum (not shown) is also aligned with the inner radio source axis, and may be due to enhanced star formation induced by the expanding radio lobes in a dense surrounding (proto-) galactic medium.

Figure 5.
(a) 1415-MHz and
(b) Lyman- α images
of 4C 41.17 at a red-
shift of $z = 3.800$.

Laser Guide Stars

Claire Max, Clifford Chocoi, and Herbert Friedman, four other LLNL collaborators, and five collaborators drawn from three UC campuses, are developing "laser guide stars" for astronomical adaptive optics. The motivation for the project is to improve the angular resolution achieved at ground-based observatories. If the project is successful, the angular resolution at major observatories might be improved by factors of 10 to 100.

The angular resolution of all ground-based telescopes with apertures larger than 10 to 20 cm is limited to about a second of arc due to turbulence in the atmosphere. In principle, one can use adaptive optics to correct for the wave front distortions with a wave front sensor, and deforming a flexible secondary mirror so as to make the wave front flat. This would allow ground-based telescopes to be operated at or near their diffraction limits. For example, at a wavelength of $0.5\ \mu\text{m}$, the diffraction-limited resolution would be 0.04 arcsec for a 3-m telescope such as that at UC's Lick Observatory and 0.01 arcsec for a 10-m telescope such as the new Keck Telescope. These represent improvements in resolution of factors of 25 and 100, respectively, relative to the atmospheric resolution of about 1 arcsec.

To accomplish this correction in the visible range, however, one needs a bright reference object within a few arc seconds of the object being imaged. The statistics of bright stars are such that at most a few percent of the sky is accessible for diffraction-limited viewing, using nearby bright stars as the wave front reference.

To make up for the lack of bright reference stars, the consortium has proposed creation of "artificial stars" using a powerful laser. Specifically, the idea is to use a laser tuned to the sodium D lines to resonantly excite the atmospheric sodium layer at 90 km altitude, making an "artificial star" to serve as a reference beacon. A wave front sensor then detects the tilts of the reference wave front, and a wave front computer uses the measured reference wave front to calculate the necessary adaptive-optics corrections. Finally, the correction is applied to a deformable mirror. The images recorded using the deformable mirror together with the telescope's primary mirror will then have most of the atmospheric distortions removed.

The hardware development aspects of the project will proceed in phases. The initial phase is a feasibility demonstration, in which a laser guide star and adaptive optics system will be implemented on a 1-m-class astronomical telescope. This system is shown schematically in Fig. 6.

Figure 6.
Proposed laser
guide star system.

Simultaneously, LLNL's laser isotope separation program will develop a high-repetition-rate laser that is compact in footprint and easily transportable to a remote site, where it can be reassembled and perform reliably and reasonably efficiently. Once feasibility has been demonstrated on a 1-m telescope, this laser will be ready to field on a 3- or 4-m system at a site such as UC's Lick Observatory.

The long-term goal is to put a laser guide-star system on the UC-Cal Tech 10-m Keck Telescope at Mauna Kea, Hawaii. The project is funded by LLNL's Institutional Research and Development Program.

A Radio Pulsar Vaporizes its Companion

A recently discovered radio pulsar (known as PSR 1744-24A) is in orbit around a "normal" star. The pulsar's radio emission is eclipsed in a complex, asymmetric fashion that cannot be explained straightforwardly by occultation by the companion star. Leigh Brookshaw and Marco Tavani have shown that the eclipses result from a strong wind of material leaving the companion star. The wind is driven by energy deposited in the surface of the star by high-energy particles emitted by the pulsar. Furthermore, the particles streaming from the pulsar exert pressure on the outgoing wind, distorting the flow and producing a highly nonsymmetric pattern of outflowing material (see Fig. 7). Brookshaw and Tavani argue that the radio eclipses are produced by this wind, thus accounting for the observations.

Figure 7. A particle plot of a model representing the pulsar vaporizing its companion star. Each dot is a particle, representing an element of gas. Dimensions are scaled by 10^{11} cm.

Center for Geosciences

The IGPP-LLNL Center for Geosciences promotes collaborative research in the earth sciences between LLNL and UC researchers. IGPP also acts as a focal point for research in the fundamental aspects of Geosciences, drawing on the expertise of scientists in LLNL's programs in national security and energy research. Our goals are to consolidate talents and capabilities at LLNL and to provide an easily identifiable avenue for LLNL-UC collaborations. Our Center is the principal physical and scientific focus for visitors from academic (UC and other universities), industrial, and government geoscience research institutions. The Center's past research emphasis has been on the physics and chemistry of the solid Earth, including seismology, geochemistry, experimental petrology, mineral physics, and hydrology. We have recently added a program in geodesy. The Center is located in and partially supported by the LLNL Earth Sciences Department, and it has strong ties with several Earth Sciences Department programs. The Center also has strong ties with the LLNL Nuclear Chemistry Division, which is a major contributor of scientific expertise and facilities for collaborative projects in geochemistry. The Center provides access to computational, experimental, and analytical research facilities and provides support in fieldwork for geophysical and geochemical studies.

Operational responsibilities for the Center are shared by George Zandt (Geophysics) and Frederick (Rick) Ryerson (Geochemistry). George is a seismologist with interests in upper mantle/crustal structure and tectonics and in the development of underground seismic imaging techniques. He currently is pursuing field projects in Northern California and in the southern Basin and Range, including Death Valley. George oversees research projects in seismology and observational geophysics. Rick is an experimental petrologist with interests in diffusion in rock-forming minerals, rheology of partially molten crustal rock, and high-pressure and high-temperature mineral-melt phase equilibria. He oversees projects in geochemistry, mineral physics, and experimental geophysics. John Rundle (formerly of Sandia National Laboratory, Albuquerque, N. Mex.) recently joined LLNL's Center. John's interests are in geodesy and the application of modern physics of complex systems to problems in the earth sciences. A portion of his time will be used to develop a geodesy program at LLNL. Geodetic measurements play an important role in constraining crust and mantle dynamics, and their use in tracing glacial advances and retreats also should influence studies of global climate variations.

Renovation and construction of new facilities during 1990 has helped the Center meet the needs of university collaborators. The Geosciences Center was completely renovated, with new office space and an "open area" that houses the Center's library and five computer workstations for visitors. Since access to the Center does not require a Q clearance, university collaborators have ready access to LLNL computer facilities. Similarly, the Nuclear Chemistry Department recently constructed a new experimental laboratory facility in an uncleared area adjacent to their main building. The new laboratory will consolidate a number of experimental facilities that currently reside in limited access areas. Included among these facilities are an ion microprobe, an electron microprobe, an ICP mass spectrometer, and several clean-lab facilities. A new facility for the preparation of accelerator mass spectrometry (AMS) samples will also be constructed in this laboratory. In addition, a portion of the main Nuclear Chemistry facility will be renovated and reclassified to provide uncleared access to the thermal ionization mass spectrometry facilities. All of these changes will greatly improve IGPP's ability to pursue collaborative research programs in geochemistry.

In 1990, Susan Beck completed her IGPP–Geosciences Postdoctoral Fellowship and accepted a faculty position at the University of Arizona. During the final year of her LLNL appointment, she and Howard Patton of the Earth Sciences Department conducted research on the source properties of aftershocks from the Loma Prieta earthquake. She also worked with George Zandt investigating the lower-crustal and upper-mantle structures in Death Valley. With Stuart Nishenko (USGS, Denver), Susan completed a study of historical earthquake recurrence patterns in South America and, with Douglas Christensen (University of Alaska), she completed a study of the 1964 Great Alaska earthquake. She also worked on two UCRP projects with Heidi Houston and Susan Schwartz (both of UC Santa Cruz). As a “participating guest,” Susan will continue to collaborate on research projects with LLNL scientists.

Kevin McKeegan, a postdoctoral researcher in the Nuclear Chemistry Division, continued his work on the genesis of oxygen isotopic anomalies in pre-solar inclusions in meteorites in conjunction with Rick Ryerson. McKeegan accepted a position at UCLA, where he and T. Mark Harrison (UCLA) will establish a new high-resolution, high-sensitivity ion microprobe facility. Kevin also has been appointed a “participating guest” at LLNL and will work with IGPP staff on collaborative research projects involving the ion probes at both institutions.

Mark Beeman, an experimental geophysicist working as a postdoctoral researcher in the Earth Sciences Department, has performed deformation experiments on synthetic crustal lithologies with and without partial melts. The research was performed with Brian Bonner, Bill Durham, and Rick Ryerson (all at LLNL–Earth Sciences), and David Kohlstedt (University of Minnesota). Mark also coauthored a UCRP proposal with John Wolfenstein (UC–Irvine) to investigate the deformation of halite single crystals as a function of trace element concentration.

Peter Goldstein, a postdoctoral researcher working with the Earth Sciences Treaty Verification Program, also resides in the IGPP Center. He collaborated with William Walter (University of Nevada, Reno) and George Zandt on using regional *P* waves from underground nuclear explosions at the Soviet test site in Kazakhstan to study both regional wave complexity and upper-mantle structure beneath the Soviet Platform.

Other frequent visitors to IGPP–Geosciences, who are not directly involved through UCRP, are: Harley Benz (USGS, Menlo Park), Charles Ammon (Penn State University), and Stanley Ruppert (Stanford University). Harley is working with George Zandt on several projects. The two completed a manuscript on seismic imaging of the deep structure of Northern California. Charles, a Ph.D. candidate at Penn State, worked with George Zandt on the Receiver Function method of crustal structure determination and on the development of nonlinear approaches to seismic tomography. Stanley, a Ph.D. student at Stanford, is working with George Zandt on the analysis of teleseismic data collected on a profile of portable seismic stations from the southern Basin and Range to the southern Colorado Plateau. Several portable stations were equipped with state-of-the-art digital recorders made available for collaborative projects through IGPP.

Research Highlights

Earthquake Source Studies including Loma Prieta Aftershocks

The March 28, 1964 Alaska earthquake ($M_w = 9.2$) is the second largest earthquake recorded. It had an aftershock length of 800 km. Body-wave inversion techniques were used to determine the spatial and temporal heterogeneities associated with the rupture of the 1964 earthquake. Deconvolved source time functions showed at least two major pulses of moment release with a duration of nearly 4 min. Susan Beck and Douglas Christensen (University of Alaska) characterized the 1964 earthquake as the failure of two asperities: the first and largest asperity ruptured from the epicentral region to 250 km SW of the epicenter and the second smaller asperity ruptured a patch 500 km SW of the epicenter.^{1,2} The spatial segmentation of the 1964 earthquake rupture corresponds to variations in the historic earthquake record, which indicates different recurrence intervals for these two segments. These results were added to our ongoing project of mapping the asperity distribution of the Aleutian-Alaska subduction zone.² A minimum of seven major asperities were located along this plate boundary. These asperities control the behavior of the stress release, and hence, the occurrence of the largest earthquakes.

Susan Beck and Stuart Nishenko³ also showed that the historic earthquake period for the Central Peru subduction zone suggests significant variations in the earthquake size during the last 400 years. A comparison of the intensity and tsunami data for historic earthquakes and events in this century indicated that at least two historic events (in 1746 and 1687) were much larger than earthquakes during this century (in 1940, 1942, 1966, and 1974). In contrast to the simple, single-asperity nature of the twentieth-century earthquakes, these older and larger events may represent multiple-asperity ruptures along the Peru subduction zone.

In a study of smaller earthquakes closer to home, Susan Beck and Howard Patton investigated the aftershocks of the October 17, 1989 Loma Prieta earthquake.⁴ Intermediate-period surface-waves recorded at regional distances are used to study the larger aftershocks of the Loma Prieta earthquake ($M_s = 7.1$). Source parameters (focal mechanism depth and seismic moment) are determined over a broad frequency range. The surface-wave source parameters allow us to assess the consistency between short-period and long-period focal mechanisms and the overall variability of the short-period first motion focal mechanisms.

Mid-Crustal Magma in the Death Valley Extended Terrain?

Recent geological research in the Death Valley extended terrain of the southern Basin and Range Province of the western United States indicates that more than 200 km of upper crustal extension has occurred during the past 10 to 15 million years. The extreme amount of crustal extension (by 300 to 400%) requires an isostatic response in a broad region that uplifts lower-crustal rocks to within 3 to 5 km

of the surface. Controversy remains in explaining how this uplift is accommodated at depth and the relative contributions of processes such as magma underplating, intracrustal intrusion, and intracrustal flow. George Zandt and Susan Beck began a study of this problem with a seismic investigation of the crust beneath Death Valley. Seismic reflection profiles collected by COCORP (the Consortium for Continental Reflection Profiling) in Death Valley show a prominent mid-crustal (15-km) reflector. This bright spot has been interpreted as partially molten material at mid-crustal depths, analogous to the magma body beneath the Rio Grande Rift in New Mexico. However, from the near-vertical reflection data alone it is not clear whether the bright spot indicates a low-velocity layer (partially molten rocks) or a high-velocity layer (a solidified sill).

Our goal in the Death Valley study is to develop and test an independent seismic method to confirm and characterize the reported mid-crustal velocity anomaly (based on a COCORP reflection profile). This new method is based on characterizing the scattering of the seismic phase that reflects off the base of the crust (the *PmP* phase). As the *PmP* wave propagates down and up through the crust, small scale vertical heterogeneity will generate scattered waves (both *P* wave reverberations and *P*-to-*S* wave conversions), which will appear on a seismogram as energy following the *PmP* arrival (the *PmP*-coda) in a time window of several seconds duration. Reflectivity synthetic seismograms computed with various possible crustal models for the Death Valley region indicate that in the distance range of 130 to 160 km, the timing, amplitude, and particle motion of the *PmP*-coda is sensitive to the nature of vertical heterogeneity in the mid- to lower crust.

To test these ideas, we recorded a large chemical explosion at the China Lake Naval Weapons Center on September 7, 1990 along a profile through Death Valley. Examination of the three-component seismograms recorded at 100- to 160-km range showed the presence of a large *PmP*-coda with significant converted shear energy, consistent with a crustal model containing high- and low-velocity layers in the mid-crust.⁵ Further detailed analysis and modeling is required. However, the large *PmP*-coda is strong evidence for a zone of significant vertical heterogeneity in the Death Valley crust, consistent with large-scale magmatic intrusion. In a broader context, the identification and characterization of vertical heterogeneity in the crust within different regional tectonic provinces, correlations with state-of-stress indicators, and structural and petrologic evidence will provide powerful constraints for models of the evolution of the continental crust.

Underground Imaging Studies

A new project funded by the Office of Basic Energy Sciences of DOE involves a collaborative effort by George Zandt, James Berryman, and John Zucca (all of LLNL), and John Vidale (UC Santa Cruz), Charles Ammon (Penn State University), and Harley Benz (USGS). The project aims to develop improved resolution seismic transmission imaging methods and apply them to the study of magmatic structures and processes in the Earth's crust and uppermost mantle. Our objectives are to improve existing tomographic algorithms by including new ray-tracing codes and feasibility constraints and to test new approaches (including nonlinear optimization) to tomography with synthetic and existing data sets. Preliminary field experiments will also be conducted to test new algorithms and approaches.

Charles Ammon and John Vidale are investigating a simulated annealing approach to seismic tomography.⁶ The approach is similar to a Monte Carlo search for the best fitting model but with a "temperature"-dependent component to occasionally select a model that does not fit the data better, thus simulating the annealing process in metals. Advantages of this approach are that it is independent of starting models, does not require computation of sensitivity matrices, and has been shown to find the global minimum. The disadvantage is that it can be computationally expensive, but recent advances in computing power appear to make this a viable approach.

George Zandt, Steve Jarpe (LLNL), and Harley Benz collected seismic data at Yucca Flats at the Nevada Test Site as a preliminary test for a field experiment to image the rubble zone created by an underground nuclear explosion. The experiment consisted of deploying portable recorders in a fan profile at a range of 1.5 km from a borehole in which a series of 100-lb chemical explosions were detonated at various depths. The target zone consisted of the rubble zone associated with three previous underground nuclear explosions located between the borehole and our fan profile. Our objective was to determine whether the rubble zone has a detectable effect on the seismic signals from the chemical explosions. Preliminary analysis of the data revealed several phases delayed by as much as 0.07 s for paths through the target zone as compared with paths outside the target zone. Assuming straight ray paths and a target width of 200 m, this delay would require a velocity reduction of up to 20% within the rubble zone.⁷

Upper-Mantle Structure Beneath the Soviet Platform

During the summer of 1988, four broadband, three-component seismic stations were installed inside the Soviet Union as part of a cooperative agreement between the Incorporated Research Institutions for Seismology (IRIS) and the Soviet Academy of Sciences. Recorded data provide a unique opportunity to study both complexities in regional wave propagation and crustal and upper-mantle structure inside the Soviet Union. Studies of regional wave complexity are needed to determine the potential nuclear test-ban monitoring capabilities of a regional network. Studies of crust and upper-mantle structure help us understand the geologic evolution of the region and have an important effect on our understanding of regional wave propagation.

In a collaborative effort, Peter Goldstein, William Walter, and George Zandt have used regional *P* waves from 11 presumed nuclear explosions at the Soviet test site in Kazakhstan to study both regional wave complexity and crust and upper-mantle structure beneath the Soviet Platform.⁸ Using a subset of the events as an array of sources, they identified four pulses during the first 15 s of the *P* waves recorded at a distance of 1500 km. These pulses are common to all the recordings despite a range in magnitude from 5.0 to 6.1 and differences in location as large as 15 km. Measurements of polarization and apparent velocity (the velocity at which a pulse appears to propagate along the horizontal direction toward the receiver) indicate that these pulses are *P* waves coming up approximately vertically at the receiver. The last of these arrivals is clearly incident at an angle closer to the vertical than that of the previous pulses.

When combined with the above observations, relative amplitudes of these pulses and their travel times strongly suggest that the observed complexity can be explained by large-scale variations in the Earth's upper mantle (depths from approximately 50 to 500 km). Through forward modeling, a one-dimensional velocity structure (Fig. 8) was obtained that provided much better agreement between observed and calculated seismograms (Fig. 9) than models previously proposed for this area, particularly for the discontinuity near 200 km. Although a number of previous studies have found evidence for the existence of a 200-km discontinuity, recent work, combining data from all over the world, has found little evidence for its existence. Our work suggests that such discontinuities exist on a regional scale.

Receiver Function Studies of Crustal Structure

A receiver function is the seismic response of a crustal velocity-depth profile to an impulsive teleseismic plane wave incident at the base of the crust (i.e., a kind of crustal Green's function). It is obtained experimentally by a deconvolution procedure applied to a three-component recording of a teleseismic *P* wave. The receiver function can then be used as data for an inversion technique to determine the crustal structure (i.e., the velocity-depth function) beneath the recording station. Charles Ammon (Penn State), George Randall (University of Nevada, Reno), and George Zandt recently published a new approach to the inversion of receiver function data,⁹ using a pseudo-Monte Carlo technique to find a family of acceptable models. We applied this technique to study the crustal structure of the Mojave Block in Southern California,¹⁰ and in the western Basin and Range,¹¹ and we initiated a collaborative field program with Stanley Ruppert (Stanford) and Susan Beck to record receiver function data in the southern Basin and Range and in the southern Colorado Plateau.

*Figure 8.
Comparison of our
preferred upper-man-
tle structure (solid
line) with models
suggested by other
workers.*

Lead Diffusion in Apatite and Zircon

During episodes of crustal partial melting, radiogenic isotopes and trace elements contained within the mineral phases making up the source rock are redistributed. Dependent upon the extent of melting and homogenization, the geochronologic (radiogenic daughter isotopes Pb^* , ^{143}Nd , ^{147}Hf) and geochemical information contained within these mineral phases may be perturbed, or, in the extreme, completely lost. With reference to accessory minerals, this information is lost if the mineral is completely consumed during partial melting or if diffusion of the element within the unmelted fraction of the mineral of interest is sufficiently rapid to allow equilibration on the time scale of the partial melting event. Alternatively, restitic minerals may be transported from the source region by the departing melt fraction and, under some circumstances, can carry information characteristic of the source region and the temperature history of crustal melting and transport. The effectiveness of any partial melting event (including melt formation, segregation, and transport, all of which are characterized by a specific temperature history) can be gauged in terms of three "fundamental accessory-phase parameters": the solubilities of the accessory phase in crustal melts, the equilibrium mineral/melt partition coefficients for the elements of interest, and the diffusivities, which govern the approach to equilibrium.

We developed with Danielle Cherniak and William Lanford (State University of New York, Albany) an ion-implantation method for introducing lead diffusion sources into the minerals zircon and apatite. Diffusion profiles are obtained using

Figure 9. Reflectivity synthetic seismograms predicted by the models in Fig. 8 and an observed seismogram (bottom trace). The synthetic seismogram constructed from our preferred model is shown directly above the observed data.

Rutherford backscattering spectroscopy (RBS), and the results are fit with an appropriate model to determine the diffusion coefficients. This approach is both simple and useful in studying diffusion over a temperature range of direct geologic interest without inordinately long annealing times.

Results for apatite over the temperature range 600 to 900°C are in good agreement with earlier results obtained by more conventional techniques at higher temperatures. Diffusion coefficients for Pb in zircon are higher than those obtained from a single experimental measurement and from estimates of Pb diffusion based on geochronologic data and U/Pb zoning in natural zircons. The most likely explanation for this disparity is sluggish annealing of radiation damage in zircon relative to apatite. This will require development of a different technique for measuring lead diffusion in zircon.

Rheology of Partially Molten Crustal Rocks

Granite magmatism is a major process in determining the constitution of the continental crust. Granite plutons form the cores of many mountain belts, and the ascent of granitic magma from either the upper mantle or lower crust into the upper crust is the primary mechanism by which heat-producing elements are redistributed. Lower crustal granulite anatexis has been suggested as a process leading to lower crustal dehydration and resulting in the formation of granulite terrains exposed in Archean cratons. Granite magmatism is also responsible for the transport of heat to the upper crust, as in the emplacement of epizonal plutons.

Geochemical studies of granites are voluminous and have led to a better understanding of differentiation trends, magma sources, etc. Yet the details of many of the physical processes involved in granitic magmatism remain problematic, controversial, or difficult to quantify because of the absence of relevant rheological data. How are granitic magmas segregated, and how efficient is the process? How do granitic magmas or magma-crystal mushes rise through the crust, and at what rate? By what process do high-viscosity melts or crystal-charged melts differentiate? How is the final emplacement depth determined, and how are the mechanics of final emplacement related to those of ascent? This project's goal is to provide rheological data relevant to the ascent of granitic diapirs (i.e., mixtures of melt and crystals) through the crust, the segregation of magma from crystals, and inversion of lower crustal seismic data.

Mark Beeman, Brian Bonner, William Durham, and Rick Ryerson (all LLNL) with David Kohlstedt (University of Minnesota) are developing methods to fabricate fine-grained aggregates of minerals and partial melts to be used in deformation experiments at elevated pressures. Current work concentrates on quartz-bearing aggregates. The sample powders are produced by spray-drying solutions or colloidal suspensions of the components. The results of these experiments are encouraging because subsequently hot-pressed samples made from colloidal silica result in quartz aggregates, while those made from metal alkoxide solutions result in glass. Hence, crystal-glass aggregates can be fabricated by mixing colloidal silica solutions with metal alkoxide solutions of the appropriate composition before spray-drying. Results of deformation experiments indicate that these samples are about an order of magnitude weaker than found in previous experiments on coarse-grained natural quartzites and are in better agreement with crustal strengths inferred from the rates of diapiric ascent of granitic magmas.

Multianvil Press

Development and use of the cubic multianvil press has continued (see the 1989 *IGPP Annual Report* for a description of the apparatus). During the past year, Rick Ryerson and Carl Boro developed the methods for fabricating furnace parts. They started experiments, with Quentin Williams and graduate student Daniel Farber (both of UC Santa Cruz), to determine the fractionation of trace and minor elements between mantle minerals and high-MgO melts known as komatiites. (The rationale for this work is described in the UCRP report by Quentin Williams below.)

Preliminary results indicate that the thermal gradients within the current furnace assembly cause chemical differentiation in the sample through a combination of thermal migration and Soret diffusion. While this process can be deleterious for some types of experiments, it may be advantageous in partitioning studies, because it results in a large homogeneous melt zone at the center of the sample surrounded by crystalline material. Analysis of the melt pool and of crystals at the interface will provide the desired partitioning data.

Oxygen Anomalies in High-Temperature Inclusions in Meteorites

Kevin McKeegan and Rick Ryerson expanded the range of oxygen diffusion data relevant to the observed oxygen isotopic anomalies in Ca, Al-rich inclusions (CAIs) in meteorites. The ^{16}O excesses in these phases result from the mixing and interaction of ^{16}O -rich interstellar material with solar nebular material (isotopically normal). Understanding the isotopic array provided by these samples will help to elucidate the composition of interstellar material available to the accreting solar nebula (and hence, the astrophysical sources that contributed to it), and also the temperature history of these inclusions within the solar nebula. This thermal history will, in turn, constrain possible nebular processes and parameters, such as dust/gas ratio, and turbulence and turbulent viscosity. Using their diffusion data as input, they developed a "dynamic crystallization/exchange model" that is capable of explaining the anomalies. The model implies the action of short-lived transient phenomena and brief high-temperature events that are much more intense than the pressures and temperatures provided by standard nebula models. The results of this work were presented at the Lunar Science Conference (March 1990) and as seminars at Cal Tech, Arizona State University, and UCLA.

Single Crystal Synthesis

High-quality single crystals of rock-forming minerals are required for many types of physical and chemical properties measurements. Particular interest is in large crystals of olivine, the major mineralogical constituent of the upper mantle. Graduate student David Hansen (University of Colorado) spent three months at LLNL, working with Morris Young and Rick Ryerson synthesizing Fe-bearing olivine using a floating-zone growth technique. This method employs an image furnace operated by the Experimental Geophysics Group. Unzoned crystals up to 7 cm long were grown. The crystals are being used in deformation experiments, and a paper describing the fabrication method is in press.

Workshops

LLNL and UC Santa Cruz cosponsored the 84th Annual Meeting of the Seismological Society of America May 2 to 4 in Santa Cruz, which was attended by 350 scientists from throughout the world. IGPP partially supported this national meeting, and the Center for Geosciences played an important role in its organization. The Seismological Society of America was founded in 1906, following the Great San Francisco earthquake, to promote research on earthquakes and earthquake engineering. It was without our planning that the timing and location of the 1990 meeting was particularly serendipitous as it occurred about six months after the 1989 Loma Prieta (Santa Cruz Mountain) earthquake and on the 85th anniversary of the 1906 San Francisco earthquake. The theme for the meeting, "Seismology for the Nineties," reflected the forward-looking role that many scientists have brought to the field. LLNL seismologists made significant contributions in areas of nuclear explosion seismology, instrumentation development, and the application of signal-processing and artificial-intelligence techniques to seismological problems.

We are proud of the role LLNL took in the organization of this national meeting as well as in our scientific contributions. Frederick Followill (LLNL) convened this meeting with Karen McNally (UCSC). Fifteen Livermore scientists, principally from the Treaty Verification Program and the IGPP Geosciences Center, contributed technical presentations; many gave multiple talks. Eight LLNL scientists chaired sessions, whose topics ranged from "Nuclear Explosion Seismology" (Steve Taylor and Marvin Denny in the Treaty Verification Division) to "Earthquake Rupture Process and Fault Zone Heterogeneity" (Susan Beck, IGPP). A session on "Weak/Strong Motion Site Effects" highlighted a talk by Stephen Jarpe and Lawrence Hutchings that examined ground motion data collected at LLNL and other Bay Area locations during a special deployment by Livermore scientists to record aftershocks of the Loma Prieta earthquake. A public evening session on "California Faults and Seismotectonics" (chaired by Frederick Followill) explored the research and policy challenges presented by California earthquakes in light of the 1989 Loma Prieta earthquake.

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Section III. Research Summaries of Collaborative Projects

High-Pressure Sciences

Shock Compaction of High- T_c Oxide Powders: The Search for a Practical High- T_c Superconductor

Principal Investigator: M. Brian Maple (UC San Diego)

LLNL Collaborators: William J. Nellis and Samuel T. Weir

Students: Christopher L. Seaman and Edward A. Early (UC San Diego)

To enable the practical application of bulk polycrystalline oxide superconductors with high critical transition temperature T_c , we have used shock compaction to "tailor" microstructural features in these oxides. The microstructure must be such as to allow high critical current density both within grains and between grains.

Abstract

Specimens are shock-compacted with the LLNL two-stage light-gas gun and are prepared and characterized at UC San Diego. Dense, crystallographically oriented high- T_c specimens with high concentrations of crystal defects have been fabricated by shock compaction of superconducting powders. Magnetic relaxation and hysteresis measurements indicate an increase in flux-pinning energies and intragranular critical current density due to shock-induced defects. Transport measurements suggest that the heat produced during shock removes oxygen at grain boundaries. Subsequent low-temperature anneals reestablish superconductivity in these regions without destroying the shock-induced defects or the crystallographic alignment.

With their unprecedentedly high superconducting critical temperatures T_c and upper critical fields H_{c2} , the newly discovered high- T_c superconducting copper-oxide materials have the potential of revolutionizing technology. As with low- T_c materials, processing-related challenges remain before bulk, high- T_c materials become available for wide practical application. The principal challenges are how to make useful forms out of these brittle ceramics and how to increase the critical current density J_c .

Objectives

Shock compaction of high- T_c powders¹⁻³ addresses three key issues that must be resolved to increase the transport J_c . (1) The primary problem in developing high transport current density in oxide superconductors is the nature of the material at grain boundaries, which limits the *intergranular* J_c . Dynamic compaction is uniquely capable of processing this region heterogeneously. Because shock compression is so fast, the compressive energy is deposited heterogeneously at the boundaries of particles that are compacted. Thus, the nature of material between grains can be varied by adjusting the pressure and duration of a shock wave used to bond powder particles. (2) Shock compaction can bond prealigned powders into a dense specimen, allowing better bonding, reducing weak superconducting links between grains, and allowing the supercurrent to flow in the basal plane of the crystal structure (the crystal orientation in which J_c is highest). (3) Shock processing

can also increase the *intragranular* J_c of high- T_c superconductors through the introduction of high densities of shock-induced dislocations and other defects that act as flux-pinning sites. Understanding the flux-pinning mechanisms in the high- T_c superconductors is also of great current scientific interest. Thus, this is a situation in which both scientific and technological goals are achieved simultaneously.

Shock-compaction research involves the use of the unique two-stage light-gas gun facilities at LLNL to fabricate shock-compacted research-size specimens under controlled conditions. The gas gun accelerates projectiles ("impactors") to velocities of 1 to 8 km/s. A high-pressure shock wave is generated by the impact of a projectile onto a target. For example, a copper projectile striking a copper target at 3.5 km/s generates a 1-Mbar shock pressure; plastic striking copper at 1 km/s generates 50 kbar. By choice of impactor velocity and material, one can generate continuously tunable shock pressure. Thus, the LLNL gas gun can be used for a wide range of material synthesis and processing experiments. A key component of the research is the use of LLNL's new, small (7 m long), 20-mm-bore gun, which produces appropriate specimens faster than earlier guns.

Progress

Our past research has demonstrated the viability of shock compaction as an important processing step in the fabrication of bulk material with high J_c . Shock treatment produces defects that increase flux-pinning energies.⁴ Magnetic relaxation and hysteresis measurements of shock-compacted $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ indicate that these defects increase the flux-pinning energy by a factor of about three, which translates into a tenfold increase in the *intragranular* J_c . Using the new Rigaku x-ray diffractometer at UCSD, we have determined the degree of alignment of the grains in shock-compacted $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$. Our results show that grains of the initial powder particles are aligned by shock compaction itself near the surface of the sample, whereas those in the interior have no preferential alignment. To obtain alignment in a larger region of the sample, we have therefore begun fabricating thin specimens of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ for shock compaction.

We have succeeded in fabricating dense, bulk high- T_c specimens of oriented $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ by shock compaction of pre-aligned powder at pressures of 30 to 150 kbar.⁵ The alignment is retained up to 150 kbar (the highest pressure attempted so far) and after subsequent heat treatments up to 800°C. Hence, there is a wide range of variables that can be "tuned" to optimize superconducting properties.

The temperature dependence of the electrical resistivity of a sample shocked to 100 kbar can be compared with that of the same shocked sample after various oxygen anneals (Fig. 10). The resistivity of the as-shocked sample (which is sensitive to the particle boundary regions) is similar to that of oxygen-deficient $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ single crystals; heat generated at the grain boundaries during the shock causes removal of oxygen from these regions, yielding lower values of T_c . We note that there is an additional change of slope with temperature for the as-shocked specimen at the magnetic superconducting onset temperature $T_c^M \approx 90$ K. A subsequent low-temperature anneal reestablishes superconductivity at the grain boundaries, without destroying the shock-induced defects in the interior of the grains, and yields specimens with high T_c (see Fig. 10). The resistivity of the 100-kbar-shocked sample after an oxygen anneal at 800°C was nearly the same as that of an unshocked, aligned, sintered pellet. The unshocked specimen, however, has a lesser degree of preferential orientation and lacks shock-induced defects that increase J_c .

This project has so far received two U.S. patents⁶ for shock synthesis and processing of superconductors and ferromagnets. A third patent is apparently about to be issued, and two other patent applications are pending. Thus, this project is concerned with both the physics and materials science of shocked high- T_c superconductors and with the potential technological applications of our results.

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Figure 10. Temperature dependence of normalized electrical resistivity of a 100-kbar-shocked $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ sample after various oxygen heat treatments, and of an unshocked, aligned, sintered pellet. The as-shocked data have been shifted vertically to emphasize differences with the other data, which are normalized to unity at 295 K. (From Ref. 2)

Shock of Preheated and Precooled Quartz

Principal Investigator: John Christie (UC Los Angeles)

LLNL Collaborators: William J. Nellis and Wayne Brocious

Student: Andrew Gratz (UC Los Angeles)

Abstract

Shocked quartz is a standard material for identifying explosive events and explosive event horizons such as the Cretaceous/Tertiary boundary; it is also a model for the general shock behavior of silicates. Using the LLNL two-stage light-gas gun facility, quartz single crystals at initial temperatures of -170 to $+1000^{\circ}\text{C}$ were shocked to pressures of 12 to 32 GPa. Shock-induced microstructural features were catalogued using the UCLA transmission electron microscope (TEM) facility and optical microscopy. Increasing pressure led to widespread brecciation and to melting and in situ vitrification. Ambient temperature has little effect on the formation of shock lamellae, but it strongly affects the formation of glass and thus the fragmentation of the sample. Transmission electron micrographs revealed a variety of lamellae types, whose individual characteristics may be diagnostic of the peak shock pressure attained. Finally, we report the first example of shock-induced dislocations in quartz.

Objectives

Shock-induced microstructures and high-pressure phase changes in minerals are fundamental in the identification and study of terrestrial impact craters and in the analysis of lunar and meteoritic samples. The discovery of shock features in quartz and feldspar from the Cretaceous/Tertiary (K/T) boundary showed that a huge explosive shock event took place at the K/T transition. The K/T transition layer in the Earth's geological record dates from the extinction of the dinosaurs and numerous other species. The purpose of this research is to shock and recover well-characterized specimens at known pressures and temperatures and to correlate the shock histories with the residual microstructures. In this way it may be possible to deduce the material history of mineral specimens from their microstructures.

Progress

Using LLNL's new 6.5-m-long two-stage light-gas gun, we shocked 16 single-crystal specimens of quartz at pressures up to 32 GPa at initial temperatures of -170 to $+1000^{\circ}\text{C}$ using specially designed heating and cooling recovery fixtures.¹ Temperature gradients were negligible in these holders, and almost all specimens were recovered intact. One experiment was followed by an ice-water quench within minutes of the impact.

Specimens as thin as $10\text{ }\mu\text{m}$ having excellent polished surfaces were prepared with a dimple grinder. These specimens were ion-milled to produce high-quality TEM foils. Samples were studied using a combination of TEM and optical microscopy. A wide range of features were observed, including fractures, microfault zones, curvilinear features, shock lamellae, microbreccia zones, and diaplectic glass.

A large number of electron micrographs showed three distinct trends with increasing pressure. First, fractures grew with increasing pressure into wide breccia zones that eventually dominated the samples. Low-pressure shocks left crystal orientations almost unchanged; although fracturing was intense, breccia zones were narrow. Breccia zones grew with increasing shock pressure until only 100- μm -sized "islands" of single-crystal quartz remained. In all samples, the breccia zones consisted of highly angular quartz (often with lamellae and other shock features) surrounded by low-density silica glass.

Second, the amount of glass increased with peak shock pressure. This glass took two forms: in shock lamellae it was in the form of diaplectic glass, and in breccia zones it was melt glass. The density of the diaplectic glass was close to that of quartz; the melt glass was considerably less dense. Some optically isotropic regions of diaplectic material were truly amorphous, but others were only cryptocrystalline. We thus infer parallel processes of *in situ* glass production (at lamellae) converting crystalline islands to glass, and of melting that progressively engulfs the islands.

Third, lamellae became more complex with increasing peak pressure. We classified lamellae into five types (see Table 2), ranging from narrow, short lamellae seen at low peak pressures to wide, complex networks seen at high peak pressures. The appearance of optically visible lamellae is correlated with the presence of Type 4 to 5 lamellae as seen in TEM. (We must use TEM to characterize the

Table 2. Lamellae types in shocked quartz.

Lamellae type	Description (from TEM)	Optically visible?
1	Short or discontinuous, narrow (tens of nanometers or less), straight in parallel sets	No
2	Long, narrow, straight, in parallel sets or networks	No
3	Long, thick (>100 nm), straight, in parallel sets, bands, or networks	No
4	Long, thick, bent and/or wedged, in networks	Yes
5	Long, thick bands of transverse lamellae or metamict material	Yes

microstructure because lamellae are optically visible only when their widths approach 0.5 μm . Figure 11 shows an example of thick, complex lamellae. Systematic study with the universal stage showed that lamellae formed at high angles to the direction of shock propagation.

Temperature had a relatively minor effect on the formation of lamellae. The highest class of lamellae observed at 24 GPa decreased from Type 5 at -170°C to Type 4 at 500°C and above. This resulted, however, in a definite decrease in the density of optically visible lamellae at higher temperatures.

On the other hand, temperature had a major effect on the amount of glass produced. At cryogenic temperatures, the 12-GPa sample barely held together because of fracture, which we interpret as a lack of glass cementing the fractures together. Samples recovered from 32 GPa progressed from largely crystalline at 20°C to completely glassy at 1000°C . Thus, the amount of glass produced at a given pressure is directly related to the initial specimen temperature.

These temperature effects have important implications for planetary processes. They indicate that significantly more comminution is to be expected on colder planetary surfaces than on the Earth, and that impact on hot surfaces (like Venus or near magma bodies and volcanoes) will produce anomalously large amounts of glass.

Figure 11. Shocked quartz seen in TEM. Thick, Type 5 shock lamellae viewed at 30,000 $\times$ show a metamict structure.

We also observed the first occurrence of shock-induced dislocations in quartz. These took the form of a dense array of crystallographically controlled dislocations (Fig. 12), formed at 24 GPa and -170°C . While these might be interpreted as signs of plastic deformation, we believe that this is unlikely under cryogenic conditions, where quartz is typically extremely hard. Instead, we note the similarity to certain dislocation arrays seen in dry quartz after apparently brittle deformation, and suggest that rapid opening and closing of microfractures may result in lattice misfits taken up by dislocation networks. We thus believe that brittle-melt deformation dominates in shocked quartz under all conditions studied.

We plan to use the remaining material and to shock more specimens to characterize the physical properties and nature of the glass and crystallites produced by the shock process.

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Figure 12. Shocked quartz seen in TEM. Densely packed, crystallographically controlled dislocations at 40,000 $\times$.

Melting and Other Phase Transitions of Simple Solids at High Pressures

Principal Investigator: Malcolm F. Nicol (UC Los Angeles)

LLNL Collaborators: David Young and Marvin C. Ross

Students: Bruce Baer and Hyunchae Cynn (UC Los Angeles)

Abstract

Melting and solid-solid phase transitions in simple solids at the high pressures characteristic of planetary interiors reflect a delicate balance between the properties of the various phases. Predictions about melting curves and other phase boundaries are very sensitive to details of statistical-mechanical models for both phases. Comparisons of measured and predicted phase boundaries can critically test statistical-mechanical models of matter compressed to these high pressures. This project couples UCLA expertise in measuring phase transitions at high pressures and LLNL expertise in modeling equations of state, especially the melting curves of molecular solids. During this year, our experiments defined the phase diagrams and reactions for several one-component systems [S_8 , HCN, and the explosive RDX (1,3,5-trinitro-1,3,5-triazocyclohexane)] and for N_2 - O_2 binary mixtures. Experiments on the sulfur system were extended to high temperatures.

Objectives

Modeling the structures of the outer envelopes of the giant planets and their satellites requires an understanding of the phase and chemical transitions of simple molecular solids. The dark species observed on comets and many satellites may result from chemical reactions among simple H-C-N-O species. Accurate measurements of these transformations at high pressures also provide sensitive tests of statistical-mechanical theories of the solid and liquid states. This project extends our determinations of phases of O_2 , N_2 , mixtures of O_2 and N_2 , S_8 , and two H-C-N-O compounds with interesting high-pressure chemistries (RDX and HCN). The experiments of the UCLA collaborators, in the diamond-anvil regime of high pressures, are designed to obtain results of accuracy high enough to challenge LLNL's theoretical models of dense fluids and solids.

Progress

The pressure-volume isotherms of N_2 - O_2 were measured up to 35 GPa for nearly the complete range of compositions.^{1,2} Baer's dissertation, completed in December 1989, studied phases of N_2 , O_2 , and their mixtures. He determined the ambient isotherm of N_2 - O_2 for a nearly complete range of compositions. Among the few simple binary systems that have been studied, N_2 - O_2 has several phases with uniquely high miscibilities in the solid state at many pressures. Among the phases identified are the following: β - N_2 , which has a P63/mmc, hexagonal structure; δ - N_2 , which has a Pm3n, cubic structure; γ - O_2 , which is isomorphous with δ - N_2 ; β - O_2 , which has a R3m structure; β - O_2 II, which has an unknown structure; δ - O_2 , which has an Fmmm structure; and ϵ - O_2 , which has a A2/m structure. In δ - N_2 , β - O_2 , and β - O_2 II, more than half of the molecules of the host crystal may be substituted by guest species. A new high-pressure variety of δ - N_2 - O_2 with up to 37% O_2 ordered at adjacent (0.5, 0.25, 0) sites was also discovered and characterized.

Several excitation wavelengths were used in studying the Raman spectra of solid S_8 compressed under N_2 .³ Discrepancies between reports in the recent literature regarding a possible new phase between 5 and 8 GPa were resolved. With 515-nm excitation, the Raman spectrum of S_8 changed near 6 GPa as if a

reversible phase transition occurred at this pressure. The strong Raman spectra of the new phase persisted well above 6 GPa. These changes were not observed under 600-nm excitation. Experiments showed that the wavelength dependence was not due to laser heating and that photochemistry was involved. We are continuing this work by studying the Raman spectra of high-temperature and high-pressure phases of sulfur, with the goal of establishing the structure of the product phase.

The phase behavior and reactivity of HCN was studied at high pressures.⁴ By visual observations and Raman spectroscopy, we determined the pressures at which HCN melts (0.2 GPa), undergoes a tetragonal-to-orthorhombic phase transition (0.8 GPa), and reacts to form a deep red polymer near ambient temperature (1.3 GPa). Samples of the polymer were recovered at ambient pressure. Fourier-transform-IR spectra showed that a new species ($N=CH$) was produced. Work is continuing on the characterization of the recovered polymer and scaleup of the synthesis to obtain samples of millimeter scale and larger.

Raman spectroscopy was used to study some nitramines and nitroaromatics at high pressures. The temperature and pressure dependence of a little-known phase transition in RDX near 3.8 GPa indicates transitions from both of these phases (designated α and γ) to a high-temperature, high-pressure RDX phase (β -RDX).^{5,6} Cynn showed that β -RDX is identical to a form of RDX known to be extremely metastable at ambient pressure, and that β -RDX is stable with respect to α -RDX and especially to γ -RDX at high pressures and temperatures. This work is being extended to other nitro-explosives.

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Design of a System to Extend Measurement of Elastic Constants up to 2000 K

Principal Investigator: Orson Anderson (UC Los Angeles)

LLNL Collaborator: Alfred Duba

Other Collaborators: Donald Isaak and Hitoshi Oda (UC Los Angeles)

Abstract

Understanding of the physics of the deep Earth requires knowledge of the elastic properties of minerals at temperatures well above the Debye temperature, above which all thermal vibrations of a crystal lattice are excited. Because the Debye temperatures of representative minerals range from 600 to 1100 K, elastic-constant data for temperatures well above 1000 K are of geophysical interest. Earlier we designed and constructed a furnace and measured elastic constants of minerals up to 1825 K. To study iron-bearing minerals at high temperatures under controlled oxygen fugacity, we have now constructed a furnace designed so that a highly reducing gas can surround and flow past the specimen.

Objectives

The absolute temperature of the deep Earth is estimated to be two or three times the absolute Debye temperature of minerals in the lower mantle. To understand the physics of the deep Earth, it is therefore important to obtain accurate elastic-constant data for representative minerals at temperatures well above the Debye temperature, which ranges up to about 1100 K for deep-Earth minerals. We built a furnace and measured the elastic constants of minerals up to 1825 K with the rectangular-parallelepiped-resonance method.¹⁻³ To study iron-oxide minerals, it will be necessary to incorporate into the furnace a system that can control the oxygen fugacity of the atmosphere surrounding the specimen.

Progress

We have constructed a system to control, at a low value, the partial pressure of oxygen at the surface of a specimen as temperature is increased in the furnace. The system uses a streaming mixture of carbon dioxide and carbon monoxide. Experiments were performed to measure the elastic constants of two different natural olivine minerals. These specimens have molecular Mg/Fe ratios of 0.90 and 0.92, respectively. A third specimen, a synthetic one produced at LLNL, was prepared with a molecular Mg/Fe ratio of 0.85. The experiments were performed up to 1600 K. Experiments could not be performed at higher temperatures because of the low signal-to-noise ratio. Future design of the apparatus will focus on minimizing the noise in the measurement system.

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Effect of Pressure on Viscosity of Ionic Liquids

Principal Investigator: Mark Bukowinski (UC Berkeley)

LLNL Collaborator: David B. Boercker

Student: Lars Stixrude (UC Berkeley)

Abstract

We previously developed a model that gives a very accurate account of the physics of crystalline and amorphous phases of tetrahedrally coordinated SiO_2 . The purpose of the current project is to apply a generalization of this model to the study of viscosity. In the past year, we have tested and developed molecular dynamics codes that compute the viscosity of a liquid. Furthermore, we have demonstrated that the topology of liquid and crystalline silica changes significantly with pressure. The changes are characterized by a positive correlation between mean ring size and density, regardless of whether the density differences are due to isobaric structural differences or to pressure differences. Pressure also is likely to cause coordination changes in the liquids. Since this involves a qualitative change in Si–O bonding, we initiated a study of the physics of this bond, with the goal of obtaining a simple, yet accurate, form of the potential that explicitly depends on bond order. At high pressures this bond is likely to be fairly ionic, so the viscosity of ionic liquids will be examined before covalent effects are included.

Objectives

Pressure can have important effects on the thermodynamics and viscosity of silicate liquids. These in turn affect the chemical and thermal evolution of the Earth. Therefore, to understand many aspects of the Earth's history, it is necessary to have information on the structure of liquid silicates and the dependence of that structure on applied pressure. There is spectroscopic evidence that coordination changes can be induced by moderate pressures, but it is not known what effect these changes have on the thermodynamic properties and viscosity of silicate liquids. It is the purpose of this project to investigate, through numerical simulations based on accurate potential models, the relation of viscosity to liquid structure, and to separate the effects of isochoric topological changes from the effects of isostructural volume changes. In particular, we want to explore the role played by structural defects (i.e., threefold-coordinated Si and nonbridging oxygens) and to find whether other structural changes are likely to occur that may affect the viscosity of liquids at high pressure.

Progress

We tested a molecular dynamics code written by David Boercker by comparing calculated viscosities with published values for the Lennard–Jones system $u(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6]$, where $u(r)$ is the Lennard–Jones intermolecular potential, ϵ is the energy scaling parameter and σ the intermolecular scaling distance. For argon, $\epsilon/k = 119.76$ K and $\sigma = 3.405$ Å. Our results are in good agreement with previous simulation values at $T^* = kT/\epsilon = 0.73$ and $N^* = N\sigma^3/V = 0.8442$, corresponding to the solid-liquid-vapor triple point, and at $T^* = 1.90$ and $N^* = 0.8010$. While existing molecular dynamics studies of viscosity have concentrated on the relatively low-pressure, low-temperature region near the triple point of argon, conditions in the earth's interior are more extreme: pressures far exceed the bulk modulus of

typical silicate liquids. Therefore, we also calculated viscosities of argon along the 800-K isotherm, corresponding to the highest measured melting temperature, from the triple point density to near the freezing density. The results, shown in Fig. 13, are in excellent agreement with the Enskog hard-sphere theory of viscosity. This suggests that for simple liquids like argon, the viscosity is determined primarily by the repulsive interactions.

The structure of silicate liquids at low and moderate pressures is dominated by the directional properties of covalent bonding, rather than by simple hard-sphere type interactions. Therefore, as a preliminary to the viscosity calculations, we sought to understand the dependence of the structural properties of tetrahedrally coordinated silica on pressure. This investigation was based on a simple, but accurate, covalent potential model of silica.¹ We found, somewhat paradoxically, that pressure increases the mean size of rings in liquids. A simple Bethe lattice model accounts for this effect, and shows that in crystalline tectosilicates as well, the framework density increases with increasing mean ring size.² This leads to a novel compression mechanism that may cause liquid-crystal density inversions even without coordination changes.³ Similar phenomena were observed in simulated SiO_2 glass at high pressure, although the changes in ring statistics were less pronounced.⁴ The model yielded a very accurate equation of state of glass; it correctly predicted irreversible densification for glass subjected to pressures of over 10 GPa, and the calculated structure was found to be in excellent agreement with available neutron and x-ray scattering experiments.

Figure 13. Viscosity calculated with our molecular dynamics code using the Green-Kubo method for argon (circles) and with the Enskog hard-sphere theory of viscosity. The effective hard-sphere diameter was determined by perturbation theory. Viscosities are scaled to the density-independent Boltzmann result $\eta_0 = (5/16\sigma^2)(mkT/\pi)^{1/2}$, where m is the atomic mass.

It has been suggested that the pressure-induced structural changes expected in silicate liquids lead to a saturation of the excess compressibility (relative to solids) and a consequent stiffening of the liquid. Our simulations of silica liquid show no evidence of this phenomenon at pressures below 50 GPa. We further tested this idea by formulating a thermodynamic model of liquids and solids in which the equation of state is assumed to be given by the Birch-Murnaghan equation. The model yields melting curves for several silicate liquids that agree very well with data at pressures higher than those at which the proposed stiffening is supposed to take place.⁵ We therefore conclude that no real evidence exists for the proposed stiffening. Data on the melting of MgSiO_3 perovskite at pressures above 100 GPa could resolve this issue. If stiffening occurs in this pressure regime, the slope of the melting curve should increase significantly. Available data extend to about 100 GPa and give no conclusive evidence for or against stiffening.

We have seen that covalent effects play a very important role in the structure, and hence the properties, of silica. These effects must be taken into account in a simulation if it is to yield reliable viscosities under variable pressure conditions. We have therefore postponed actual simulations until we believe we understand the structural effects. Simulations of ionic liquids will be performed as additional tests of the codes. The results of these simulations will have a bearing on silicate liquids at high pressure, but they may not shed much light on the pressure effects on viscosity at upper mantle conditions. Since this is where most important magmatic effects take place, the covalent effects are likely to be most important. We therefore plan to concentrate on covalent structural effects and on the proper means to simulate them with the molecular dynamics code.

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High-Pressure Investigation of Charge- or Spin-Density Waves in $\text{Sc}_5\text{Co}_4\text{Si}_{10}$ -Type Compounds

Principal Investigator: Robert N. Shelton (UC Davis)

LLNL Collaborators: Harry B. Radousky and Robin L. Reichlin

Students: John Dykes, Tim Goodwin, and William D. Mosley (UC Davis)

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Abstract

The interplay between the superconducting or magnetic state and the charge-density wave (CDW) or spin-density wave (SDW) formation in $\text{Sc}_5\text{Co}_4\text{Si}_{10}$ -type compounds can be studied using high-pressure magnetic susceptibility and electrical resistivity measurements. The effect on superconductivity of the suppression of the CDW/SDW ratio is being examined for the compound $\text{Lu}_5\text{Rh}_4\text{Si}_{10}$. Similarly, the effect of the CDW/SDW ratio on the magnetic properties of the nonsuperconducting compound $\text{Tm}_5\text{Ir}_4\text{Si}_{10}$ is being studied and compared with the corresponding effect in isostructural superconducting compounds.

Objectives

The suppression of the CDW/SDW ratio in $\text{Sc}_5\text{Co}_4\text{Si}_{10}$ -type compounds with applied hydrostatic pressure can be observed with both magnetic susceptibility and electrical resistivity measurements. The suppression of the CDW/SDW in the material is accompanied by a sudden increase in the superconducting transition temperature (measured by susceptibility) at some pressure. Similarly, resistivity measurements show the depression of an anomaly in the electrical resistance to lower temperatures. Utilizing these two techniques, namely susceptibility and resistivity, and the application of pressure, one could completely determine the temperature-pressure phase diagram of the superconducting and magnetic states for $\text{Lu}_5\text{Rh}_4\text{Si}_{10}$ and $\text{Tm}_5\text{Ir}_4\text{Si}_{10}$.

Progress

A significant part of this project continues to be the development of a method for resistivity and susceptibility measurements for use with the diamond anvil cell (DAC). In collaboration with LLNL, we explored techniques for measuring the resistivity of small samples at high pressures. The collaboration has given us a starting point for measurements of resistivity on small samples in the DAC. In addition, the techniques discussed provide considerable insight into using the DAC to obtain high pressures. Facilities for pressure calibration using the ruby fluorescence have not been set up at UC Davis, limiting further development of the resistivity techniques at high pressures.

We are adapting an rf method for measuring the susceptibilities of small samples (volume = 10^{-8} cm^3) for use in the DAC. The method uses two parallel resonant circuits operating at high frequencies (3 MHz) to detect changes in the sample

susceptibility. A parallel inductor-capacitor circuit is operated at its resonant frequency. The inductor is a wound coil containing the sample. The highly tuned circuit is sensitive to changes in the inductance of the sample coil. When the sample becomes superconducting, the diamagnetism changes the coil inductance and thereby changes the resonant frequency of the circuit. The frequency shift is converted to a voltage that is proportional to the susceptibility.

To test the sensitivity of this method, we built a simple probe for dipping in liquid cryogenics consisting of a coil holder, a heater, and a thermometer. This design allows testing of various coil configurations. Sensitivity calculations based on our *rf* circuit design indicate that the circuit should have sufficient sensitivity to measure a superconducting transition from a sample with a volume of 10^{-8} cm^3 . Additional problems related to background noise must be eliminated to provide optimum sensitivity.

The temperature-pressure phase diagram for $\text{Lu}_5\text{Rh}_4\text{Si}_{10}$ and $\text{Tm}_5\text{Ir}_4\text{Si}_{10}$ is being investigated. The development of the susceptibility detection circuit will enable us to complete the measurements.

Theoretical Search for Metastable Structures of Light-Metal Hydrides

Principal Investigator: Ching-Yao Fong (UC Davis)

LLNL Collaborators: Andrew McMahon and Christian Mailhot

Student: Robert Gallup (UC Davis)

Abstract

We have investigated the electronic, structural, and mechanical properties of two possible metastable phases of beryllium hydride, BeH_2 , using total energy calculations based on the self-consistent pseudopotential and linear muffin-tin orbital methods. The structures are the fluorite and calcium carbide structures, which contain one and two BeH_2 formula unit per primitive cell, respectively. Both phases are semimetals with ionic bonding between the negatively charged hydrogen ions and the positively charged beryllium ions. The bulk modulus for the fluorite structure is three times higher than that of the calcium carbide structure, whereas the energy content of the calcium carbide structure is significantly greater than that of the fluorite structure. Both phases may be accessible from the observed BeH_2 structure by the application of pressure.

Objectives

The solid phases of the light-metal hydrides (LMHs) have recently been proposed as potentially convenient and efficient hydrogen storage systems that could be used as energy sources. Even though few stable solid phases of hydrogen-rich LMHs have been discovered in normal temperature and pressure environments, they might be formed under high temperature or pressure and returned to ambient conditions as metastable states. Certainly the complexity of the observed structure of BeH_2 and those of the many allotropes of elemental boron are suggestive of such metastable states. Furthermore, the metastable states of these materials may result in additional energy content—a desirable attribute for an energy storage system. The purpose of this study is to investigate the electronic, structural, and mechanical properties of possible metastable phases of one LMH (BeH_2) using total energy calculations based on the self-consistent pseudopotential and linear muffin-tin orbital methods. Information obtained from this study can provide guidance for subsequent experimental attempts to synthesize these materials.

Progress

Two possible metastable structures of BeH_2 have been investigated. The first, the fluorite structure, is based on a face-centered cubic lattice and contains one formula unit per primitive cell. The second, the calcium carbide (CaC) structure, is based on a body-centered tetragonal lattice and contains two formula units per primitive unit cell. One major difference between these two structures is the distance between neighboring hydrogen atoms: the hydrogens are more widely separated in the fluorite structure than in the CaC structure.

The variation of total energy with the volume per BeH_2 unit has been calculated for both structures. The bulk moduli of both structures were deduced from the energy-vs-volume curves by fitting the calculated results to the Murnaghan equation of state. We found that the bulk modulus of the fluorite structure (0.29 Mbar) is three times higher than that for the CaC structure (0.09 Mbar).

The electronic properties for the room-pressure volumes of both structures have also been calculated. The electronic band structures indicate that BeH_2 is a semimetal in both structures. The self-consistent charge densities predict, however, that both of these phases are partially ionic—the valence electrons from the beryllium are transferred to the hydrogens (Fig. 14). In addition, the hydrogens in the CaC structure appear to form H_2^{2-} ions. However, the CaC structure has a significantly higher room-pressure energy than the fluorite structure. This result indicates that the negatively charged hydrogen ions prefer to be spatially separated, and suggests that molecular hydrogen ions do not contribute to the hydrogen content in the beryllium hydrides.

During this investigation, we have extended our self-consistent computer codes to enable us to study nonsymmorphic structures with more than 40 atoms per unit cell. We are performing calculations for the observed BeH_2 structure, which contains 36 atoms/unit cell.

Finally, although the energy content of a possible metastable structure can be determined with our total energy computer codes, dynamic simulations are needed to ascertain whether a given structure is metastable. We are implementing a Car–Parrinello molecular dynamics computer code to determine the stability of possible metastable structures.

Figure 14. Charge-density contours of the full valence band in a (110) plane for BeH_2 in the fluorite structure, showing the transfer of charge from the beryllium atoms (squares) to the hydrogen atoms (circles).

Experimental and Theoretical Studies of Metal Under Pressure

Principal Investigator: Raymond Jeanloz (UC Berkeley)

LLNL Collaborator: J. A. Moriarty

Student: Charles Meade (UC Berkeley)

Other Collaborator: B. K. Godwal (UC Berkeley)

Abstract

The metals molybdenum and rhenium, which have been proposed or used as calibration standards for experiments at static ultrahigh pressures, exhibit unusual properties under compression. Shock-wave and ultrasonic data, in combination with new first-principles quantum mechanical calculations, indicate that changes in the electronic bonding configuration of Mo lead to increased compressibility and perhaps to an anomalous increase in rigidity with increasing pressure. With this understanding, it is possible to construct an internally consistent equation of state for molybdenum that supports the use of this metal as a pressure-calibration standard.¹ Rhenium, in contrast, is found to be a poor calibration standard despite the fact that the electronic bonding configuration of this metal is in theory relatively insensitive to pressure. Specifically, new measurements of the yield strength of Re to static pressures exceeding 100 GPa show that strength effects can seriously bias measurements of the equation of state of this metal.²

Objectives

The goal of this project is to combine state-of-the-art experimental and theoretical techniques to investigate the properties of metals under pressure. Because changes in pressure can significantly alter the bonding in metals, there is considerable interest, both fundamental and practical, in using pressure to expand our understanding of material properties. Comparisons of experimental measurements with predictions obtained from first-principles quantum-mechanical calculations allow us to interpret observed changes in material properties in terms of the underlying changes in electronic structure. We also want to assess quantitatively the utility of a given metal as a component of experiments: for example, as a calibration standard or as a high-strength material.

Progress

The equations of state of body-centered-cubic (bcc) solid and of liquid molybdenum were calculated to pressure-temperature conditions of 600 GPa and 14,000 K by means of the linear muffin-tin orbital (LMTO) method and the corrected rigid-ion sphere (CRIS) model. Our results agree with previous work in documenting a pressure-induced shift of valence electrons from the 5s to the 4d states, especially at pressures above 100 GPa. An analysis of ultrasonic and shock-wave measurements, together with our theoretical results, demonstrates that the compressibility of bcc Mo is increased at pressures of 100 to 200 GPa. The increased compressibility, and possibly an anomalous increase in rigidity suggested by previous sound-velocity measurements in shock-compressed states, are caused by the pressure-induced transfer from s to d states. Our study further substantiates the use of the Mo equation of state as a calibration standard for ultrahigh-pressure static experiments and, in particular, supports the prior calibration of the ruby-fluorescence standard.

In contrast, LMTO calculations for rhenium in its hcp phase show virtually no change in electronic structure over the pressure interval 0 to 300 GPa. Furthermore, the electronic contribution to the shock-wave equation of state is negligible over this pressure range, suggesting that rhenium might be a useful calibration standard as well. However, this conclusion is not supported by new measurements of static yield strength.

We measured the strength of Re to 120 GPa, by far the highest static pressures of any yield strength measurements to date, and found that rhenium can sustain shear stresses of up to ~ 10 GPa at room temperature. These are the highest shear stresses ever observed in such studies, thus reinforcing previous conclusions that Re is an exceptionally strong component for high-pressure experiments. Though high in absolute value, the strength of rhenium is not anomalously high according to theoretical micro-mechanical predictions that scale yield strength to the shear modulus. The equation of state obtained by conventional axial-geometry x-ray diffraction through the diamond cell is biased, however, because of the high strength of Re. The amount of bias serves as a secondary estimate of yield strength, and agrees quantitatively with the primary estimate obtained from measurements of pressure gradients across the sample. The bias in the equation of state of Re measured in ultrahigh-pressure static experiments precludes the use of this metal as a reliable calibration standard.

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Collaborative Analysis of Gamma Ray Burst Energy Spectra

Principal Investigator: Kevin C. Hurley (Space Sciences Laboratory,
UC Berkeley)

LLNL Collaborators: Edison Liang and Charles Dermer

Cosmic gamma ray bursts are short pulses of high-energy radiation, whose origin is only very poorly understood. To gain insight into the physical processes that generate the gamma radiation, we initiated a systematic study of gamma-burst energy spectra. Our goal was to compare state-of-the-art theoretical models, constructed at LLNL, with a large experimental data base, from the Franco-Soviet SIGNE experiments aboard Venera 13 and 14 and Prognoz 9. We have nearly completed the software development for this project and have found a surprising and potentially very significant result in the preliminary analysis of a portion of the data. This is a close correlation between the intensity of a gamma-ray burst and the effective temperature of its spectrum. Such a correlation can be interpreted to yield information about burst energization mechanisms. We have also studied the time profiles of gamma-ray bursts, and we have found a diagnostic tool for determining whether such bursters are in binary systems. Detailed studies of radiation processes occurring on highly magnetized neutron stars lead us to propose a functional form, $L \propto (kT)^n$, to fit gamma-ray burst spectra.

Abstract

Several lines of evidence point towards galactic neutron stars as the sources of gamma ray bursts. Still, many fundamental facts remain obscure. One essential element is the energization process that converts mechanical, gravitational, or rotational energy on or about the neutron star to gamma radiation. A clue to the nature of this mechanism can be found by studying the spectra of gamma bursts. Bremsstrahlung, synchrotron, Compton, and pair-annihilation processes leave their signatures in burst energy spectra, and by studying the observed spectra, we can, in principle, determine which of these processes is dominant. At LLNL, a relativistic plasma radiation code has been developed for the study of relativistic Maxwellian electrons of arbitrary temperature and density in the presence of a magnetic field of arbitrary strength. We also have developed a numerical code for calculating the photon spectrum produced when electrons lose energy by Compton-scattering photons in a superstrong magnetic field. One goal is to apply the results of these codes to a large data base on cosmic gamma-ray bursts in a rigorously correct manner. That is, we use the code to generate model spectra that are folded through the detector response function; these theoretically predicted spectra are then compared with the observed spectra.

Another goal of our work is to better understand the time profiles, or light curves, of bursts. Are they correlated in any way with the energy spectra? Is there any simple interpretation of their shapes?

Objectives

Progress

We have almost completed the software effort required to treat the entire data base of approximately 200 gamma-ray bursts (each of which may, on the average, have 10 to 100 half-second energy spectra recorded at different intervals) in a routine, production fashion. When this is accomplished, we will subject each energy spectrum to a detailed analysis, comparing the observed spectrum with model spectra generated by the LLNL code. We have begun this analysis for a selected set of intense bursts and have found a quite unexpected result. For a given event, we have analyzed the energy spectra taken at various times throughout the burst using a simple optically thin thermal bremsstrahlung fit; the important free parameter in this procedure is the effective temperature kT . We have repeated the analysis for approximately six bursts, and in each case have found that the burst intensity is strongly correlated with kT . The data are consistent with a relation in which the luminosity L is proportional to $(kT)^n$, where $n \approx 1.5$. Figures 15 and 16 illustrate this effect for one event. If this finding is confirmed, such a relation will have important implications for the energization model.

In a related study, we have considered the possibility that gamma-burst light curves, or time histories, may contain clues to a binary origin of bursters.¹ We call this effect an "x-ray echo." Such an echo originates when the gamma radiation from a neutron star impinges on a nondegenerate binary companion. A fraction of the gamma radiation is scattered by the companion's atmosphere and emerges as a weaker, softer-spectrum echo of the main gamma burst. To identify possible echoes, we have examined the data of the Venera 11, 12, 13, and 14 gamma burst experiments. We conclude that these detectors were at the limit of the sensitivity required to detect echoes, but that detectors in operation over the next year or so, aboard the Gamma Ray Observatory, will have enough sensitivity to detect and identify echoes and thus possibly determine the binary nature of bursters.

Figure 15. Time history of the November 4, 1982 gamma-ray burst, in the 50–950-keV energy range.

Finally, we have undertaken a systematic analysis of the process of Compton scattering of photons by energetic nonthermal electrons in superstrong magnetic fields.² These fields are a trillion times stronger than the Earth's magnetic field and are thought to occur on neutron stars. This analysis solves a number of problems about gamma-ray burst spectra and how gamma rays can escape from the surface of a neutron star without being degraded by pair-producing interactions with the intense magnetic field. It also suggests a new functional form for fitting gamma-ray spectra that we are implementing in our studies of gamma-ray burst spectra. This study will help shed light on the acceleration mechanisms operating in gamma-ray burst sources.

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Figure 16. Temperature–luminosity correlation for the burst of Fig. 15. The kT was found by fitting a function proportional to $(1/E) \exp(E/kT)$ to the observed five-channel energy spectra for 33 time intervals in the burst. The luminosity varies as $L \propto (kT)^n$, where $n = 1.78$ (solid line). The correlation coefficient $r = 0.91$.

A Survey of the Galactic Plane at 327, 1400, and 5000 MHz

Principal Investigator: Robert Becker (UC Davis)

LLNL Collaborator: Eric Keto

Other Collaborators: S. Zoonematkermani (student, Columbia University),
D. Hepland (Columbia University), and R. White (Space Tel. Sci. Inst.)

Abstract

The 1400-MHz Very Large Array (VLA) Radio Telescope survey of the galactic plane resulted in a catalog of 1990 discrete sources. These sources were spatially divided into two distinct components: (1) Population I sources with a very narrow distribution in galactic latitude (typically within 25 pc of the galactic plane) and (2) extragalactic sources with a uniform distribution. The Population I sources are very young objects. They often appear in the Infrared Astronomy Satellite Point Source Catalog and are primarily compact and ultra-compact ionized hydrogen (H II) regions. The radio data provide the best available census of these objects.

Objectives

The purpose of this research is to obtain an accurate picture of the structure of our Galaxy and to quantify rates of star formation and supernovae. This is best achieved at radio wavelengths, where there is little or no obscuration. The intent is to image the Galaxy at three wavelengths, each of which is necessary because different classes of objects have their own spectral signatures and can be more readily observed at different wavelengths. The 1400-MHz survey was ideal for detecting optically thin H II regions. This fall and winter (1990–1991) the 5000-MHz survey will be made; its goal will be to observe optically thick H II regions. Eventually, the 327-MHz survey will be used to search for supernova remnants.

Progress

This year the 1400-MHz survey was completed and three manuscripts prepared. Zoonematkermani et al.¹ presented the catalog of sources, Becker et al.² discussed their spatial distribution, and White et al.³ discussed the IR properties of the sources.

We have demonstrated the presence of an extreme Population I component with a scale height of 25 pc restricted to within 50° longitude of the galactic center.² This scale height is significantly less than that normally given for O stars, 60 pc. For the first time, we are seeing the true distribution at which massive stars are formed; this assumes that these radio sources are compact H II regions and that they are present only at the earliest stages of an O star's existence. Presumably, the O stars subsequently disperse to greater distances off the galactic plane (60 pc) before blowing up.

It was also shown that, indeed, the *Infrared Astronomy Satellite* (IRAS) colors of the Population I objects are consistent with those of compact H II regions.³ (Figure 17 shows the IRAS colors of the IRAS counterparts to the radio sources. The region of the figure in which compact H II regions are found is indicated.) We also note that while the IRAS data cannot distinguish compact H II regions from embedded B stars, the radio data can. This ambiguity in the IRAS data has previously prevented researchers from accurately measuring the density and distribution of O stars.

The success of this survey has resulted in the award of VLA observing time from the National Radio Astronomy Observatory for completion of the 5000-MHz survey in late 1990. A follow-on program of observations of specific sources revealed in the survey is planned for the Berkeley-Illinois-Maryland Millimeter Array. This work constituted the Ph.D. thesis of S. Zoonematkernani.

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Figure 17. Colors of IRAS counterparts of the Galactic Plane Survey radio sources. Typical colors of ultracompact H II regions, planetary nebulae (PN), and red giant stars (RG) are indicated. $F(\lambda)$ refers to measured flux density at wavelength λ .

Multi-Object Spectroscopy on the 40-in. and 120-in. Telescopes at Lick Observatory

Principal Investigator: Jean P. Brodie (UC Santa Cruz)

LLNL Collaborators: Charles Hailey, Jay Bixler, and Kem Cook

Other Collaborator: William Craig (UC Berkeley)

Student: Ralph Hanks Donnelly (UC Santa Cruz)

Abstract

Over the past three years, an automated fiber-optic multiobject spectrograph (AMOS) has been developed for use in the 40-in. and 120-in. telescopes at the Lick Observatory. During FY 90, AMOS was taken out of the laboratory and used successfully on the 40-in. telescope.

Objectives

The primary objective during FY 90 was to install the multiobject spectrograph on the 40-in. telescope at Lick Observatory. This would serve to test the instrument under normal operating conditions, to demonstrate the viability of the design, and to begin acquisition of scientific data.

Progress

The multiobject positioning system was constructed and extensively tested in the laboratory and at the 40-in. telescope.¹ The engineering testing phase at the 40-in. is close to completion, and the device will henceforward be used on a regular basis for scientific data collection. Initially, scientific programs will be carried out on the 40-in. telescope. The move to the instrument's final destination, the prime focus of the 120-in. telescope, has been postponed because of delays in the manufacture of the wide-field optical corrector required to provide the 1° field of view at that telescope. Delays have also occurred during the past year because of the late arrival of parts for the spectrograph and initial problems with the commercial CCD detector.

A new spectrograph has been brought into operation that can accommodate up to 55 fibers. To date 15 fibers have been used simultaneously with this spectrograph, and 11 more fibers will be included for the next observing run.

The guiding and acquisition systems were considerably improved during the year. The target assignment and anti-collision algorithms were optimized. The ability to compensate for temperature variations was introduced. A variety of methods for assembling fiber housing buttons to the required accuracy were investigated, and a highly reliable and repeatable method was developed for batch production. The spectrograph has been assembled, aligned, and calibrated, and the CCD detector was received, characterized, and brought into operation.

The following are the results of the laboratory and telescope tests: (1) The positioning system places fibers to an accuracy of $\leq 10 \mu\text{m}$ at all orientations with respect to gravity. (2) The acquisition system can acquire objects down to about the 14th magnitude on the 40-in. The purchase of a new intensifier is expected to improve this limit by two to three magnitudes. (3) The guide system currently operates down to the 12th magnitude on the 40-in. The system's relay optics have been redesigned and, once the new optics have been installed, a guide limit of about 15.5 magnitude is anticipated. (4) The total system efficiency is about 16%, including the telescope, at $6500 \text{ \AA}$. (5) Fiber-to-fiber variations are $\ll 10\%$.

The instrument meets or exceeds design goal specifications and is ready for scientific data collection.

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The Cosmic Quark-Hadron Transition and Primordial Nucleosynthesis

Principal Investigator: George M. Fuller (UC San Diego)

LLNL Collaborators: Charles R. Alcock, David Dearborn, Grant J.

Mathews, Bradley S. Meyer, Robert Malaney, and Hannu Kurki-Suonio

Students: Karsten Jedamzyk and Yongzhong Qian (UC San Diego)

Abstract

We have investigated how density fluctuations generated in a cosmic quark-hadron phase transition might have altered primordial nucleosynthesis yields relative to those of the standard, homogeneous Big Bang. Nucleosynthesis calculations have been performed that implicitly couple neutron diffusion and nuclear reactions. Additionally, we have made a preliminary calculation of neutrino and photon "inflation" and hydrodynamic expansion of the fluctuations against Thomson drag, and have estimated the effects of these processes on primordial nucleosynthesis yields. We find that some inhomogeneous models for the Big Bang could significantly extend the limit on the baryonic contribution to the closure density Ω_b to $\Omega_b = 0.2$ to 0.4 , although $\Omega_b = 1$ is ruled out due to ${}^4\text{He}$ overproduction. In addition, our calculations show that hydrodynamic expansion of the fluctuation can reduce the ${}^7\text{Li}$ yield in inhomogeneous primordial nucleosynthesis by several orders of magnitude over previous calculations, possibly reducing the ${}^7\text{Li}$ production below that in the standard Big Bang. We have investigated intermediate-mass element synthesis in these models and have explored nucleosynthetic "signatures" of inhomogeneity at the nucleosynthesis epoch.

Objectives

Comparison of observed abundances of the light elements with calculations of corresponding primordial nucleosynthesis abundance yields is the only known probe of the physics of the very early universe ($T > 10$ keV). For the standard homogeneous Big Bang, this comparison¹ yields a limit on the baryonic contribution to the closure density of about $\Omega_b = 0.16/h^2$ (where h is the Hubble constant in units of $100 \text{ km s}^{-1} \text{ Mpc}^{-1}$). In contrast, it has been pointed out that cosmic vacuum phase transitions (such as a QCD transition) before the nucleosynthesis epoch might generate isothermal baryon number fluctuations. These fluctuations are modified by neutron, proton, and photon diffusive and hydrodynamic processes, so that the universe is inhomogeneous in baryon number density and neutron-to-proton ratio during the nucleosynthesis epoch. These processes modify the nucleosynthesis yields.² It is difficult to calculate the nucleosynthesis yields in these inhomogeneous models, however, because the processes that modify the fluctuation amplitudes and geometries may proceed on time scales comparable to, or shorter than, the actual nucleosynthesis time scale. Our primary objective was to develop a nucleosynthesis code that implicitly couples nuclear reactions with the modification processes so that we can calculate the abundance yields from a variety of plausible initial fluctuation characteristics. Ultimately, we hope that abundance observations can be used to constrain the inhomogeneity of the universe at the nucleosynthesis epoch, which in turn may yield important constraints on the QCD epoch. We also wanted to know what the limit on Ω_b would be in inhomogeneous models.

We have mapped out³ the primordial nucleosynthetic yields for the light elements as a function of initial baryon-number-fluctuation characteristics, the mean co-moving separation of fluctuation centers, and Ω_b . These calculations include implicit coupling of neutron diffusion and nuclear reactions in 16 to 32 spatial zones per fluctuation site. The conclusions are that, although $\Omega_b = 1$ is ruled out because of helium over-production, the acceptable "limit" on Ω_b ($\Omega_b \leq 0.3h^2$) is considerably higher in the inhomogeneous models than in the standard Big Bang. This is a significant increase in the allowed baryonic content of the universe, because it may allow baryons to make up all of the dynamically inferred dark matter ($\Omega = 0.2h^2$ to $0.3h^2$) in clusters of galaxies. Furthermore, we note a characteristic feature of inhomogeneous cosmologies, namely that the ^4He abundance is usually less than that in the standard model for a given Ω_b . We suggest that the primordial ^4He abundance may be one of the best diagnostics of primordial inhomogeneity. These results are summarized in Fig. 18.

Figure 18. (a) Mass fraction Y_p of ^4He vs mass fraction Ω_b of baryons in the universe for a typical inhomogeneous model (solid line) and the standard Big Bang (dotted line). Boxes indicate observational limits. (b) Number ratios of D , ^3He , and ^7Li , relative to ^1H vs Ω_b , for a typical inhomogeneous model (solid line) and the standard Big Bang (dotted line). Boxes indicate observational limits.

We have carried out calculations of photon-diffusive expansions of the fluctuations from the end of the QCD epoch ($T \approx 100$ MeV) through the end of primordial nucleosynthesis ($T \leq 10$ keV), and we have found that the damping of the fluctuations becomes rapid once the photon mean free path becomes comparable to the length scale of the high-density regions of the fluctuations. This rapid expansion sets in near $T = 20$ to 50 keV and can result in considerable destruction of ${}^7\text{Be}$, and hence of ${}^7\text{Li}$. We have made simple estimates of the effects of coupled hydrodynamics and nuclear reactions in this regime.⁴ We conclude that the ${}^7\text{Li}$ abundance is difficult to characterize in inhomogeneous cosmologies, and that for large-amplitude fluctuations it may actually be lower than in the standard Big Bang.

We have studied the yields of intermediate-mass elements in low- and high-density regions in inhomogeneous cosmologies.⁵ Finally, we have studied the nucleation process during a putative first-order QCD-epoch phase transition to determine what the distribution of nucleation-site length scales should be.⁶

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The Berkeley Mid-Infrared (IR) Array Camera and the Nuclei of the IR Bright Galaxies

Principal Investigator: John Arens (Space Sciences Laboratory, UC Berkeley)

LLNL Collaborators: Eric Keto and Roger Ball

Student: Margaret Meixner (UC Berkeley)

We have begun a study of a newly discovered class of galaxies whose nuclear regions emit strongly in the infrared. IGPP funding helped support two series of observations at the NASA Infrared Telescope Facility. The observations suggest that the infrared emission may be due to a burst of star format in a very small region. The scale of this region approaches that of the nuclei of active galaxies.

Abstract

The IR bright galaxies discovered by the Infrared Astronomy Satellite (IRAS) are significant in the context of the evolution of starburst galaxies, active galaxies, and quasars. These galaxies are distinguished observationally by very high luminosities (approaching that of quasars) and by a high ratio of far-IR to total luminosity. The latter observation implies that these galaxies emit nearly all of their extreme power in the far-IR. Ground-based IR observations, which achieve higher angular resolution at shorter wavelengths than the IRAS satellite, show that the IR activity at the wavelengths of these observations is localized in a small region around the galactic nuclei. The extent of the brightest emission is found on a scale below the previously available instrumental resolution, typically 2 to 4 arcsec in the mid-IR and 0.5 to 1 arcsec in the near-IR, or within several hundred to a thousand parsecs around the galactic nuclei at a distance of 50 Mpc. The small spatial scales observed in galactic nuclei suggest that the IR bright galaxies may be similar to quasars in that these galaxies emit an extraordinary amount of energy from an extraordinarily small region of space. Thus, determining the size of the emission region is an interesting scientific objective that may bear on the origin of quasars and the evolution of galaxies over cosmic time.

Objectives

The unique capabilities of the Berkeley mid-IR array camera, developed at the Space Sciences Laboratory of UC Berkeley and jointly operated with IGPP-LLNL, allow imaging the morphology of the mid-IR emission on the scale of 100 pc. This constrains the mid-IR emission region to a diameter one-eighth as large as that previously known. Our results¹ show that the starburst galaxy NGC1614 (Fig. 19) contains a double structure in the nuclear region. Most of the flux (78% of 655 ± 50 mJy) is emitted in two unresolved regions of 0.6 arcsec FWHM (190 pc at 64 Mpc) of nearly equal strength separated by 0.625 arcsec (200 pc). Most of the remaining flux is derived from a small arm about 1 arcsec (310 pc) in length. The Seyfert 1 galaxy NGC7469 (Fig. 20) shows an elongated structure, unresolved in the minor axis, 1 arcsec (320 pc at 66 Mpc), but clearly extended in the major axis, 2.5 arcsec (800 pc).

Progress

Several papers have suggested, in the more general context of active galactic nuclei and starbursts, that galaxy collisions may be responsible for the triggering of extreme activity in the nuclei or starbursts. In a normal galaxy, the disk structure is a manifestation of the balance between centrifugal and gravitational forces. A collision of two galaxies previously in equilibrium will result in a new distribution of energy and angular momentum about the new center of mass of the colliding pair. Gas and stars with low energy and angular momentum in the new system will collapse, while material with higher energy and angular momentum will be ejected.

Many of the IR bright galaxies show the signatures of such interactions, long streams of stars extending from an asymmetric or disrupted disk and exceptionally dense concentrations of stars and gas about the galactic nuclei.

Our observations are significant in this context, revealing that the emission in the galactic nuclei may be attributable in some cases to a burst of star formation on a scale much smaller than previously thought possible, approaching the scale typically associated with active galactic nuclei.^{1,2} Thus some phenomena ascribed to active galactic nuclei may be better understood as a star burst.

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Figure 19. Image of the nucleus of NGC1614 at $12.5\ \mu\text{m}$. The ticks at $0.5\ \text{arcsec}$ intervals correspond to about $160\ \text{pc}$ at $64\ \text{Mpc}$ ($H_0 = 75$). The angular resolution is about $0.5\ \text{arcsec}$.

Figure 20. Image of the nucleus of NGC7469 at $12.5\ \mu\text{m}$. The ticks at $0.5\ \text{arcsec}$ intervals correspond to about $160\ \text{pc}$ at $66\ \text{Mpc}$ ($H_0 = 75$). The angular resolution is about $1.1\ \text{arcsec}$.

Relativistic Shock Waves in Synchrotron Sources

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LLNL Collaborators: Masahiro Hoshino, A. Bruce Langdon,
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Student: Yves Gallant (UC Berkeley)

Abstract

We have used both analytic theory and particle-in-cell computer simulations to study the structure of relativistic shock waves in electron-positron and electron-positron-proton plasmas. The results indicate that shocks with weakly magnetized upstream flows can be good candidates for the machine that accelerates relativistic, nonthermal particles in astrophysical synchrotron sources, if the flow is composed of electrons, positrons, and a low-number-density admixture of heavy ions. When the heavy ions provide the dominant energy density in the flow, the downstream plasma has a power-law distribution of positrons in energy space, $N(E) \propto E^{-2}$. In contrast, shocks in pure pair plasmas are completely thermalized downstream. These results are the first direct evidence that relativistic shock waves can account for the nonthermal energy observed in astrophysical synchrotron sources.

Objectives

The intellectual focus of the research lies in the attempt to understand the origin of nonthermal energy in astrophysical systems. The research goal during the FY 89 grant period was to study the basic physics of relativistic shock waves, with a view toward application to the origin of synchrotron emission in supernova remnants powered by pulsars and to the emission from jets emanating from active galactic nuclei. This work made use of existing LLNL plasma simulation codes, whose properties are ideally suited to studying the electromagnetic phenomena associated with these shocks.

Progress

Our work on the structure and particle acceleration properties of relativistic shocks made substantial progress during the past year. We completed our one-dimensional studies of pure electron-positron shocks with the magnetic field polarized across the flow. We demonstrated that the results depend almost exclusively on the upstream ratio σ of the Poynting flux to the kinetic energy flux ($\sigma^{1/2}$ is also the ratio of the upstream relativistic cyclotron frequency to the relativistic plasma frequency).

The downstream wave spectra and energy density have been measured and shown to be well described as a Rayleigh-Jeans spectrum, with intensity at the level expected for the downstream temperature. We also showed that the downstream particle distribution function is Maxwellian. Thus, a form of "violent relaxation" has brought the downstream plasma to a state closely resembling thermal equilibrium for a relativistic, two-dimensional gas. Therefore, transverse magnetosonic shock waves in a pure electron-positron plasma cannot by themselves be the origin of the nonthermal particle spectra observed in synchrotron sources.

We identified the dissipation process operative in the one-dimensional models as a synchrotron maser. This was done by studying the linear instability of cold relativistic rings in a homogeneous plasma. We also followed the development of the instability with uniform, periodic electromagnetic simulations to identify the characteristic spectra and distribution functions produced. These were found to be very similar to the wave spectra and particle distributions found downstream from the one-dimensional shock simulations, thus suggesting the dissipation process in the

shocks to be synchrotron maser activity in the inhomogeneous magnetic field of the shock front. Because much of the spectrum lies at frequencies well above the upper hybrid frequency of the downstream medium, a substantial fraction of this radiation may escape to infinity, affording the possibility of directly observing these shocks in sufficiently strongly magnetized media.

While these results may lead to some interesting astrophysics in systems where thermal electron-positron plasmas may exist, such as in quasars, they show clearly that transverse electron-positron shocks are not the source of the nonthermal particle spectra seen in plerions, where the shocks certainly should be extremely close to orthogonal to the relativistic winds flowing out of the central pulsars. The most interesting possibility in terms of the energetics is that the wind flow has a heavy ion component. Such heavy ion components are also thought to be present in quasars. This suggests considering shocks with a "proton" component of the upstream flow, in addition to the electrons and positrons.

We have carried out one-dimensional simulations of shocks with cold electrons, positrons, and protons in the upstream medium. The most interesting results occur when the protons form a small minority component of the plasma (by number), but nevertheless, dominate the kinetic energy flux. Because the protons have a much larger Larmor radius than the electrons and positrons, the pairs first form a preliminary shock, with structure essentially the same as when the protons are absent. The protons then form the dominant shock, with the dissipation coming from synchrotron maser emission of extraordinary modes by the protons. However, in the immediate post-shock region, the high harmonics in the proton synchrotron spectrum are preferentially synchrotron absorbed by the positrons, since the protons radiate left-handed, elliptically polarized extraordinary modes whose electric vector rotates in the same sense as the positrons' cyclotron gyration. This absorption process leads to the formation of a "core-halo" distribution of positrons—the positron distribution function is a Maxwellian up to energies a few times the temperature, but at higher energies it becomes a power law. When the protons have the dominant energy density, this power law is of the form $N(E) \propto E^{-2}$, where $N(E)dE$ is the number of particles with total energy between E and $E + dE$, independent of the upstream values of σ and the flow γ . The conversion of proton flow energy into nonthermal positron energy is close to 100% efficient. The spectral slope steepens and the efficiency declines as a function of decreasing energy density in upstream protons, once this energy density is at values comparable to or smaller than the energy density in pairs.

These studies have provided the first evidence that relativistic transverse shocks can create the synchrotron sources seen in plerions and at the termination shocks of jets, with the emitting particles positrons rather than electrons and the upstream flow including heavy ions. A major goal of the work in the coming year will be to apply these results to a model of the excitation of the Crab Nebula and other plerionic synchrotron sources.^{1,2}

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Horizontal Branch Stars as a Tool for Particle Astrophysics

Principal Investigator: Joseph I. Silk (UC Berkeley)

LLNL Collaborator: David P. Dearborn

Co-Investigators: Georg Raffelt and Pierre Salati (UC Berkeley)

Detailed modeling of the late stages of stellar evolution has been used to investigate the properties of various proposed elementary particles. These new particles, often known as "cosmons," can have significant influence on energy transport within stars. In this project we effectively used stars as cosmic "particle physics laboratories."

Abstract

The objective of this research was to determine the impact of cosmions on the late stages in stellar evolution, and then to use observations of stars to constrain the physical properties of the cosmion^s.

Objectives

We studied the effect of cosmion energy transfer on horizontal branch stars.^{1,2} If enough cosmions are accreted to break convection in the cores of these stars by virtue of their high efficiency of energy transfer, thermal pulses develop. That is, the star does not settle in a stationary state of equilibrium, but oscillates between phases of quiescent contraction on the Kelvin-Helmholtz time scale, and phases of violent helium burning with episodes of convection. Observationally, this would result in an increased dispersion of the horizontal branch of globular clusters and a shift to higher luminosities, which would lead to an overestimate of the age of globular clusters. In other words, the previously determined apparent ages of globular clusters may be overestimates. Also, the observed period fluctuations of many RR Lyrae stars can be explained, in principle, by these cosmion-induced thermal pulses.³ These thermal pulses can be understood analytically as oscillations of thermal relaxation between the small, energy-generating "nuclear core" of the star, and the remainder of the core, which plays the role of a "gravo-thermal buffer." If cosmions prevent convection, the former stable fixed point of convective equilibrium of the nonlinear stellar structure equations is replaced by a limit cycle with no stable fixed point. The pulses are a manifestation of the limit cycle.

Progress

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Model Spectra of Cosmic X-Ray Sources

Principal Investigator: Steven M. Kahn (UC Berkeley)

LLNL Collaborators: William H. Goldstein and Albert L. Osterheld

Student: Duane A. Liedahl (UC Berkeley)

Abstract

Atomic modeling tools developed at LLNL for use in the interpretation of x-ray spectra from laboratory plasmas have been adapted for application to several important astrophysical problems. Primary attention has been given to Fe L-shell transitions, which are prominent in the soft x-ray spectra of a wide variety of cosmic sources. We have concentrated on cases in which severe departures from collisional equilibrium are expected, particularly x-ray photoionized nebulae (present in accretion-powered sources) and ionizing plasmas (present in young supernova remnants). In each case, we have discovered discrete spectroscopic signatures of the departure from equilibrium conditions and have developed useful density and temperature diagnostics for application to measured spectra.

Objectives

Soft x-ray spectroscopy can be a powerful probe of the extreme environments associated with a remarkably diverse assortment of astronomical objects, ranging from the hot (10^7 to 10^8 K), tenuous (10^{-3} cm $^{-3}$) plasmas found in galaxy clusters to the relatively cool (10^4 to 10^5 K), dense ($>10^{11}$ cm $^{-3}$) plasmas found in the accretion disks of x-ray binaries. Relatively little has emerged from this field because of the limitations of available instrumentation, but the next series of x-ray satellite experiments will provide several orders of magnitude improvements in both sensitivity and spectral resolution for this kind of work. These new observational capabilities stimulated renewed interest in the development of discrete x-ray spectral models, which are required for the interpretation of the measured spectra. Although several plasma-emission codes are in standard use in the community, they are all based on the assumption of strict collisional equilibrium, which renders them inapplicable to many important astrophysical situations. Proper modeling of such nonequilibrium cases requires detailed accounting of all discrete atomic processes that can feed and deplete the relevant quantum levels. This can only be accomplished through the use of sophisticated atomic codes. Our approach is to search for and calibrate discrete spectroscopic diagnostics that are useful for characterizing physical conditions in diverse astronomical environments.

Progress

We have completed atomic models for most of the ions that contribute to the soft x-ray band (5 to 45 Å). These include low-temperature models ($\sim 10^5$ K, appropriate to x-ray photoionized nebulae) for Fe XVI–XXVI, O VII–VIII, Ne IX–X, and Si XIII–XIV, and high-temperature models ($T > 10^6$ K) for Fe XVI–XXVI. A model for a given ion at a given temperature consists of the atomic structure through principal quantum number 4 or 5, radiative transition rates (E1, E2, M1, and M2) connecting all levels, electron-impact excitation rates connecting all levels, photoionization and collisional ionization rates, radiative recombination rates, and, in some cases, dielectronic recombination rates.

For the case of x-ray photoionized nebulae, the electron temperature is too low to collisionally excite x-ray emitting levels.^{1,2} Radiative recombination, with an inverse temperature dependence, is the predominant excitation mechanism. Recombination-dominated population kinetics increase the populations of levels at the bottom of the cascades. We have shown that for Fe L-shell ions, this has the effect of making line ratios of the form $(3s-2p)/(3d-2p)$ significantly higher than those expected for plasmas in collisional equilibrium.³ These ratios provide a qualitative signature for discriminating between photoionized and collisional plasmas. We also discovered temperature and density diagnostics for the photoionized case. Because the electron temperature is low, the recombination L-continua are narrow ($\lambda/\Delta\lambda \approx 100$). Since the widths and continuum jumps associated with these features are temperature-sensitive, the ratio of continuum intensity at the edge to the intensity of any of the strong lines provides an excellent temperature diagnostic. Density diagnostics are associated with the presence of low-lying metastable states in the ground configurations of most of the Fe L ions. At high density ($n > 10^{13} \text{ cm}^{-3}$), the metastable states are appreciably populated and act as sources for excited states through radiative recombination. This leads to "new" lines, which emerge only at high density (see Fig. 21).

Figure 21. Density dependence of the L-shell transitions for nitrogen-like iron (Fe XX) in conditions representative of x-ray photoionized nebulae. (a) Intensity vs wavelength for $n = 10^{11} \text{ cm}^{-3}$. (b) $n = 10^{14} \text{ cm}^{-3}$. Note the forest of lines that emerge at high density. Since these lines are produced by recombination, the effect is associated with the presence of many low-lying metastable states near the ground state of the carbon-like ion.

In young supernova remnants, the x-ray emitting plasmas are underionized because time scales for electron collisional ionization exceed those for dynamical evolution of the shock front. Clear measurement of the departures from ionization equilibrium can provide very important information regarding the thermal history of the gas. We have discovered a new Fe L-shell diagnostic that allows simultaneous determination of both the electron temperature T and a particular ion ratio, $R = \text{Fe XVI}/\text{Fe XVII}$. In an underionized plasma, the Fe XVII $2p^53s$ states are populated both by L-shell ionization of Fe XVI and by cascade following collisional excitation from the Fe XVII ground state. Since collisional ionization and excitation have different temperature dependences, the flux ratios of Fe XVII $(3s-2p)/(3d-2p)$ lines depend both on T and R . Ratios of Fe XVI $3d-2p$ lines to those of Fe XVII also depend on T and R . Thus these two constraints together uniquely determine both parameters. This diagnostic technique is especially applicable to the remnant of SN1006, which is believed to be in its Fe XVI phase in the reverse shock.

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Geosciences

Stable Lead Isotope and Rare-Earth-Element Tracers of Contaminants in the Marine Environment

Principal Investigator: A. Russell Flegal (UC Santa Cruz)

LLNL Collaborators: Sidney Niemeyer and G. Price Russ III

Other Collaborators: David Garrison (UC Santa Cruz) and James Estes (U.S. Fish and Wildlife Service)

Students: Peter Ritson, Donald Smith, and Steen Trump (UC Santa Cruz)

Stable lead isotopes may be used to identify and trace anthropogenic inputs of contaminant lead in the environment. Our previous studies demonstrated anthropogenic fluxes of industrial lead aerosols to surface waters in the Great Lakes and the offshore transport of industrial lead in upwelling filaments in the Northeast Pacific. We expanded the application of these stable lead isotopic tracer techniques to investigate the cycling of lead in the marine biosphere. This includes analyses of the lead concentration and isotopic composition of preindustrial and contemporary sea otters from a remote Alaskan island and from California coastal waters. Disequilibrium in lead isotopic composition between plankton and surface waters in a Northeast Pacific upwelling regime was also resolved. Finally, preliminary analyses of rare-earth elements of marine sediments was begun.

Abstract

The principal objective of this research is to establish the validity and applicability of stable lead isotopic tracers in the environment. Our preliminary research was focused on simple systems, where pronounced differences in lead isotopic composition were predicted. Work consisted of analyses of surface waters that received discrete inputs of contaminant lead from industrial sources with distinct isotopic compositions in coastal waters off California^{1,2} and in the Great Lakes.³ The high sensitivity and precision obtained in those analyses indicated that stable lead isotopes also could be used to identify and trace the biogeochemical cycling of lead in more complex systems. Therefore, this research effort focused on the cycling of lead in marine organisms to evaluate preliminary models of biomagnification and biopurification in food chains and to quantify lead contamination in marine organisms.

Objectives

Three studies using lead isotopic tracers to investigate the cycling of lead in the marine biosphere were completed. The first study measured lead concentrations and stable isotopic compositions in the teeth of industrial and contemporary sea otters (*Enhydra lutris*) from Amchitka Island, Alaska to determine the lead contamination in marine organisms from a relatively pristine environment.⁴ The second study was expanded to include sea otters from off California, where there are point source inputs and where the sum of industrial lead inputs is substantially larger.⁵ The third study addressed the apparent isotopic disequilibrium between phytoplankton and surface waters in a Northeast Pacific upwelling filament.² Finally, we began a study of rare-earth distributions in marine sediments using inductively coupled plasma mass spectrometry analyses.⁶

Progress

The two studies of lead contamination in sea otters showed that the bioaccumulation of lead in preindustrial organisms was derived from fluvial inputs associated with the weathering of local geological formations, in contrast to the industrial origins of lead in contemporary organisms. This is illustrated by the plots of lead isotopic compositions in otters from Amchitka Island (Fig. 22). The lead isotopic composition of preindustrial sea otter teeth is the same as that of the lead found naturally in the Aleutian arc, while the contemporary sea otters contained a mixture of natural Aleutian arc lead and industrial lead from Japan, Canada, and the United States. The physical transport processes accounting for the introduction of contaminant lead to that remote location are illustrated in Fig. 23.

Results from the study of lead isotopic composition in plankton within an upwelling regime were surprising. While theoretical calculations and empirical measurements demonstrate that there is no physical, chemical, or biological isotopic fractionation of lead within the biosphere, our data indicated isotopic disequilibrium between plankton and their seawater media. This was resolved with species composition analyses and biophysical transport models, which indicate that plankton from different populations were entrained in the upwelling filament. While biologists have suggested that coastal waters contained such discrete assemblages, these isotopic analyses provided the first chemical measure of their presence.

Figure 22. (a) $^{208}\text{Pb}/^{206}\text{Pb}$ vs $^{207}\text{Pb}/^{206}\text{Pb}$ and (b) $^{207}\text{Pb}/^{204}\text{Pb}$ vs $^{206}\text{Pb}/^{204}\text{Pb}$ of preindustrial and contemporary sea otters from Amchitka Island, Alaska. Error bars in (a) are $\pm 2\sigma$. Error bars in (b) were omitted for clarity, although they were typically ± 1.5 times the symbol diameter for the contemporary sea otters and ± 4 times the symbol diameter for the preindustrial sea otters. Lead isotopic compositions of natural and anthropogenic sources are plotted for comparison. Data from M. Morozumi (pers. comm.). The Northern Hemisphere reference line is included in (b) for reference.

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Figure 23. Lead sources to Amchitka Island sea otters ($^{208}\text{Pb}/^{206}\text{Pb}$ ratios). Leads in the preindustrial otters (2.04) were derived from natural weathering of the Aleutian arc lavas (2.04). In contrast, leads in the contemporary otters (2.09) were derived primarily from Asian (left arrow, 2.12) and western Canadian (right arrow, 2.07) industrial leads that were introduced into ocean surface waters via eolian deposition.

A Study of the Re-Os Isotope System in Black Shales

Principal Investigator: John T. Wasson (UC Los Angeles)

LLNL Collaborators: G. Price Russ III and Sidney Niemeyer

Other Collaborators: L. Zhou and A. Du (UC Los Angeles)

Abstract

Separation techniques have been developed for the extraction of rhenium and osmium from black shales. The preferential enrichment of Re relative to Os in continental rocks and derived sediment should allow the $^{187}\text{Os}/^{186}\text{Os}$ ratio of sedimentary rocks to be used as an indicator of continental weathering rates.

Objectives

This project considered two different but related studies in black shale. The first involved determination of the age of Re- and Os-rich black shales deposited near the Precambrian-Cambrian boundary at Zunyi, China some 570 million years ago. Due to their very high Re/Os ratios and ages determined from other methods, moderately good precision measurements of the $^{187}\text{Os}/^{186}\text{Os}$ ratio should yield ages of this boundary that are more precise than any previously published.

Our second investigation involved the study of recent black shales to determine how the seawater $^{187}\text{Os}/^{186}\text{Os}$ ratio has varied with time. Re is strongly fractionated from Os during crust/mantle differentiation, yielding relatively high values of Re/Os and, hence, high values of $^{187}\text{Os}/^{186}\text{Os}$ in the crust. Therefore, it is plausible that temporal variations of the rate of continental weathering resulted in variations in this ratio in sedimentary rocks. If this is shown to be correct, the variations in the ratio can be used as a climate proxy.

Progress

Initial effort concentrated on developing the chemical procedures for the separation of Re and Os with high recovery and minimal contamination. L. Zhou was involved in the initial aspects of the work. Later A. Du led the work on the chemical separation procedure. The procedure developed is similar to that of Walker,¹ but the researchers also included the addition of an acetone extraction to aid the main separation of Re from Os. Experiments were performed to optimize the Os recovery by various distillation and condensation conditions. Walker's procedure did not seem to work well for extraction of Os from black shales. Black shales contain much more organic matter than most terrestrial rocks and meteorites, and this might have produced the observed problems.

Problems involving isotopic equilibration between the Os isotopic spike and the sample observed in earlier work on iron meteorites appears to have been largely resolved by our current methods of sample preparation.

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Rare-Earth Elements as Geochemical Indicators of Marine Depositional Environments

Principal Investigator: David L. Jones (UC Berkeley)

LLNL Collaborators: Marilyn R. Buchholtz-ten Brink,
David C. Gerlach, and G. Price Russ III

Student: Richard W. Murray (UC Berkeley)

Abstract

The purpose of this research is to characterize the depositional environment of marine sedimentary rocks using elements with chemistries sensitive to variations in depositional setting. The abundances of these elements act as indicators of the depositional environment, thereby facilitating their use in tectonic reconstructions. Samples of 160 ocean sediments from a variety of depositional settings were analyzed to further calibrate previous conclusions based on analyses of their lithified equivalents and to study the effects of diagenesis on sediment chemistry.

Objectives

The purpose of this research is to characterize the depositional environment of marine sedimentary rocks using elements whose chemistries are sensitive to variations in depositional setting, e.g., rates of sedimentation, water chemistry, and oxidation state. The depositional setting of a sedimentary rock is a fundamental aspect of its history and, because sedimentary rocks are contained in most tectonic sequences is a vital piece of information in plate tectonic reconstructions. For many marine sediments, such as cherts and shales, common petrographic and physical approaches alone cannot rigorously specify the depositional environment. The primary objective of this work is to determine whether the depositional setting of such lithologies can be deduced from their rare-earth-element (REE) and trace-element geochemistry. In previous years, we have focused on the chemistry of lithified sediments. To gain a better understanding of chemical changes during diagenesis, we are now focusing on the analysis of recent oceanic sediments from different depositional settings. We hope to gain a fundamental understanding of the incorporation of REEs in sedimentary rocks by examining the partitioning of REEs between contemporary marine sediments and their coexisting pore waters.

Progress

Our research concentrated on the analysis of 160 chert and siliceous sediment samples. Eighty of these samples were from DSDP/ODP (Deep Sea Drilling Project/Ocean Drilling Project) cores distributed throughout the world's ocean basins (Fig. 24). Data from these samples, though not fully interpreted, further calibrate our previous results on terrestrially exposed cherts.

The remaining 80 analyzed samples are from the Japan Sea. ODP Leg 127 drilled four sites within two basins of the Japan Sea, an isolated back-arc basin of the Western Pacific (Fig. 25). Richard Murray, a shipboard scientific participant on the Leg, extensively sampled cores drilled at the four locations. Such closely spaced sampling allows detailed assessment of the paleo-oceanographic, diagenetic, and depositional environmental sources to sediment within a relatively enclosed basin. Preliminary results suggest that diagenetic processes do not uniformly affect chemical distributions through the sediment column. Major-element variations correlate well with lithologic changes, while trace-element compositions are controlled primarily by oceanographic parameters, which are recorded between sediments of different types.

Figure 24. Locations of Deep Sea Drilling Project/Ocean Drilling Program cores analyzed during this study.

Figure 25.
Locations of Ocean
Drilling Program
Leg 127 cores from
the Japan Sea.

Experimental Rheology of Magma

Principal Investigator: Frank J. Spera (UC Santa Barbara)

LLNL Collaborators: Homer Weed and Frederick Ryerson

Student: Daniel J. Stein (UC Santa Barbara)

Abstract

We continued our rheometric investigation of magmatic and analog melt-plus-vapor emulsions by concentric cylinder viscometry. The viscosity of mixtures of GeO_2 melt containing from 0.8 to 5.5 vol% air bubbles has been measured between 1100 and 1175°C at 1 kPa in a rotating-rod viscometer at shear rates 0.05 and 7 s^{-1} . The presence of deforming bubbles in these emulsions produces measurable non-Newtonian behavior, including pseudoplasticity (shear-thinning) and the introduction of nonzero normal stress differences. There is strong variation of the relative emulsion viscosity with bubble volume fraction in strong flow fields in which bubble deformation is large relative to that in weaker flow fields. Because of these and similar effects, inferences regarding the viscosity of magmas from lava flow morphology may be incorrect if based on Newtonian behavior.

Objectives

Natural magmas are multiphase mixtures of solids and vapor bubbles dispersed within a continuous silicate melt phase. Although silicate melt viscosity varies with temperature, pressure, composition, and other variables, its variability is simpler to describe than the often complex behavior observed in nature. Among the complications observed in multiphase magmas are: yield phenomena, pseudoplasticity, thixotropy, and viscoelasticity. Sparse experimental data exist on the rheometric properties of magmatic emulsions (mixtures of melt plus vapor) despite the observation that volatile saturation is virtually ubiquitous in magma bodies from shallow depths to the surface. An important theoretical and practical goal in geophysical fluid dynamics is the development of a constitutive relation for magmas that accounts for variations due to crystallinity and bubble content and the effects of temperature, pressure, and composition.

Progress

Emulsions differ dynamically from suspensions of solids. In addition to the disturbance of flow due to the presence of a dispersed phase, forces involved in bubble deformation must be considered in the equation of motion. The relevant variables are shear rate $\dot{\gamma}$, bubble radius r , the viscosities of emulsion, melt, and vapor phases η_e , η_m , and η_v , respectively, and the melt-vapor interfacial tension σ . Parameters that characterize the rheological behavior of emulsions include the bubble volume fraction ϕ , the capillary number $\text{Ca} \equiv \eta_m \dot{\gamma} r / \sigma$, and the viscosity ratio $\lambda \equiv \eta_v / \eta_m$. The capillary number represents the relative importance of shear forces, which deform the bubbles and interfacial forces, which tend to keep them spherical. The relative viscosity $\eta_r \equiv \eta_e / \eta_m$ is a convenient way to summarize effects produced by the presence of the dispersed phase.

The effects of bubble volume fraction and changes in bubble deformation with shear rate must be considered in analyzing the rheological behavior of these emulsions. Data obtained thus far permit a tentative correlation of relative viscosity and

bubble volume fraction given by $\eta_r = 1 + 13.1\phi$ (Fig. 26). We attribute the strong variation of η_r with ϕ in our correlation to the effects of bubble deformation not present experimentally or theoretically accounted for in other studies of emulsions summarized by the other correlations shown in Fig. 26. At similar solids loadings in suspensions, the effect on relative viscosity is far smaller.

When the range of shear rates examined is large enough (a factor of 20 or more) to make a precise determination, the emulsions may be modeled by a power-law rheological model, $\eta_e = m\dot{\gamma}^{n-1}$, displaying pseudoplastic (shear-thinning) behavior, with a flow index n around 0.9 at constant bubble volume fraction. Smaller ranges of shear rate do not permit precise determination of power law parameters.⁵ In our experiments, shear rate ranges for emulsions determined to be pseudoplastic were 0.05 to 7 s⁻¹.

Bubble deformation in concentric-cylinder experiments on magmatic emulsions produces the Weissenberg effect (rod-climb), a manifestation of nonzero normal stress differences not present in Newtonian fluids. An estimate of the first normal stress difference ($N_1 \equiv \tau_{\theta\theta} - \tau_{\phi\phi}$) was made from measurements of rod climb in these experiments. It was found to be about 2% of the total shear stress $\tau_{\theta\phi}$ at shear rates of less than 10 s⁻¹ at viscosities around 10⁵ Pa·s. In more fluid lavas, normal stress differences could amount to more than 25% of the shear stress and could strongly influence the velocity field within magmatic flows. Inferences about the dynamics of lava flows may be misleading if viscoelastic effects induced by deforming vesicles are not taken into consideration.

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Figure 26. Relative viscosity vs volume fraction of bubbles for germanium dioxide emulsions; comparison with theoretical studies of dilute emulsions of nondeforming particles² and experimental studies of nondeforming particles. Error bars for the present study represent one standard deviation variation at constant volume fraction, with best fit line ($\eta_r = 1 + 13.1\phi$) forced through $\eta_r = 1$.

Quantitative Analysis of High-Frequency Seismic Polarizations

Principal Investigator: Jonathan Berger (UC San Diego)

LLNL Collaborator: Albert Smith

Students: Richard Aster and Jennifer Scott (UC San Diego)

Abstract

The proposed use of high-frequency seismic stations for improved seismic monitoring capabilities raises the issue of the effect of near-station structure on the interpretation of high-frequency three-component seismograms. In a collaborative project between LLNL-IGPP and UCSD-IGPP, we investigated the effects of source mechanisms, anisotropy, and scattering from geologic and topographic structures on the polarization of seismic energy. High-frequency three-component seismograms from an array in Southern California were used to investigate how high-frequency waves propagate in a heterogeneous, isotropic crust. Our work shows that analysis of the polarization information contained in three-component data yields strong constraints on near-station scattering effects and will thus help separate these effects from other attenuation phenomena.

Objectives

The polarization of seismic waves is a standard tool in seismic monitoring techniques employing three-component recordings. It is usually assumed that body waves are characterized by linear polarization and surface waves by elliptical polarization, and the polarization filtering gives a useful estimate of the source back azimuth. These assumptions may not be valid at high frequencies because simple source and wave-propagation models fail. In addition, one of the critical aspects of wave propagation in the context of seismic verification of nuclear treaties is that of seismic attenuation. At high frequencies, this problem is compounded by the increased importance of scattering by inhomogeneities near the sources along the path and near the seismic station.

Our main objective is to understand high-frequency seismic wave propagation effects using data from the Anza array.¹ High-frequency seismic signals from underground nuclear explosions have been shown to propagate to large distances in the Soviet Union. An understanding of these signals will therefore be important in any seismic treaty verification program.

Progress

We developed an inversion scheme to determine three-dimensional variations in seismic velocity structure from travel-time data and used it to study the upper crust surrounding the San Jacinto fault zone in Southern California. The method uses the three-dimensional ray tracing algorithm of Um and Thurber.² The velocity model is required to be smooth in the sense that the first derivative of the velocity functional is minimized, subject to the constraint that the travel-time data is fitted to within the picking errors. Earthquake hypocenters are simultaneously determined using a projection algorithm that makes the problem computationally feasible for large data sets. The method was applied to a data set of 5600 *P*-wave arrival times recorded at the 10 stations of the Anza network and 13 stations of the Cal Tech-USGS Southern California Network region of relatively homogeneous surface geology. Lateral velocity variations of 6% are required at a depth of 6 km to fit the data. This contrast

occurs in a narrow range in the fault zone, but some localized variations away from the fault can be almost twice as large. The resulting perturbations of the ray paths at the receivers can be up to 12° . We are examining the effect of different smoothness constraints on the velocity structure and the resultant seismic ray paths to determine the range of variation in polarizations expected at the receivers. We are also evaluating the necessity of site delays and their magnitude.

We completed and published an analysis of near-vertically incident shear waves to quantify seismic anisotropy in the Southern California batholith using newly developed quantitative and unbiased techniques.³ These techniques show that initial shear-wave polarizations at several stations in the Anza network are clearly aligned. These alignments are probably due to seismic anisotropy, because they are not predicted by event focal mechanisms and isotropic ray tracing. Scattering plays a significant role in altering these high-frequency signals, even in the very early *S*-wave coda. As a result, identification of a distinct slow quasi-shear wave is difficult in these data. Identification of sets of similar wave forms from events in nearly the same place but separated by up to six years provide strong evidence that the earth response is stable on the time scale of several years, even in this very tectonically active area.

An analysis⁴ of data from 300-m deep boreholes installed by the USGS⁵ near two of the Anza station sites shows that the initial shear-wave polarization alignment observed at the surface is also visible in recordings made below the weathered zone. This finding rules out the weathered zone as a principal contributor to the shear-wave anisotropy. As with the surface recordings, distinct slow quasi-shear wave phases are generally not observed, even at 300 m. Analysis of spectral ratios from different borehole levels reveals extremely high attenuation averaged over the upper 150 m ($Q_\alpha \approx Q_\beta \approx 5$). As a result of this high-attenuation boundary layer, reflected phases from the free surface and from the near-surface velocity gradient do not appreciably complicate the signals recorded downhole.

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Structure and Tectonics of the Cape Mendocino Triple Junction

Principal Investigator: John Vidale (UC Santa Cruz)

LLNL Collaborator: George Zandt

Other Collaborator: Heidi Houston (UC Santa Cruz)

Abstract

We have relocated earthquakes near the Mendocino Triple Junction where the Pacific, North American, and Gorda plates meet. Earthquake locations are significantly improved by using a dipping structure to model the subduction zone, by using the L1 norm, and by identifying and excluding noisy data. Our best locations reveal (1) the extreme flatness of the seismicity associated with the subduction thrust plane, (2) the transition from a thin zone of seismicity west of 124° W longitude to a more diffuse zone of seismicity to the east, (3) the presence of a seaward-dipping zone of seismicity above about 15 km depth at 124.2° W, and (4) a small zone of intense seismicity just offshore of Cape Mendocino that is associated with the buckling of the southern edge of the Gorda plate against the thicker and more rigid Pacific plate.

Objectives

The junction of the Gorda, Pacific, and North American plates (the Mendocino Triple Junction MTJ) occurs near Cape Mendocino, Calif. (Fig. 27). The MTJ is the intersection of the three major faults: the right-lateral strike-slip San Andreas fault, the left-lateral Mendocino transform fault, and the thrust-style Gorda subduction zone. The northward migration of this triple junction controls the development of the major tectonic features of the region. It appears possible that major earthquakes can occur on all three faults and within the plates. Current scientific opinion, while not unanimous, holds that the Gorda subduction zone and its northwest extension, the Juan de Fuca subduction zone, are both active and may have the potential for a magnitude 8 or 9 earthquake. Recent geological investigations around Humboldt Bay indicate that large earthquakes occurred on reverse faults during Holocene time. The study of current seismicity is therefore important in deciphering the complex structure of the region and its implication for earthquake hazards.

The Humboldt Bay Seismic Network (HBSN), operated for the Pacific Gas and Electric Company by TERA Corporation, recorded 14,000 earthquakes from 1974 to 1984. The network was situated off the Mendocino Triple Junction, with good coverage to the north and some coverage to the south of the triple junction. The seismicity data were assembled by Robert McPhearson (Humboldt State University), who found hypocentral locations using the program HYPO71¹ (based on a one-dimensional crustal model) and studied the state of stress inferred from focal mechanisms determined from first motions. Our first objective is to relocate the earthquakes with a more realistic velocity model taking into account the dipping structure associated with the subduction zone.

Figure 27. Location of study area near Cape Mendocino, Northern California. Boxes enclose areas of east-west seismicity cross section (Fig. 28) and north-south cross section (Fig. 29).

Progress

We relocated seismicity near the Mendocino Triple Junction using QUAKE3D,² which uses the travel-time calculation algorithm of Vidale.^{3,4} The earthquake locations are significantly improved by using a dipping structure, by using the L1 norm, and by identifying and excluding noisy data. Figure 28 illustrates the variations between the seismicity patterns produced using HYPOINVERSE (D. Oppenheimer, personal communication, 1989), using QUAKE3D with a flat-layered structure, and using QUAKE3D with a dipping-layered structure. The planar alignment of seismicity that dips gently to the east coincides with the subducting Gorda plate.

Our best locations, shown at the bottom of Fig. 28, reveal the extreme flatness of the seismicity associated with the thrust plane, the transition from a thin zone of seismicity west of 124° W longitude to a more diffuse zone of seismicity to the east, and the presence of a seaward-dipping zone of seismicity above about 15 km depth at 124.2° W. Previous workers suggested a double seismic zone or a diffuse layer of seismicity. Our more precise locations show a single, thin sheet of seismicity. Focal mechanisms in the Gorda plate change from N-S compression west of 124° W longitude to down-dip tension to the east, roughly coincident with the

Figure 28. East-West cross section of seismicity (40.6 to 41°N) with hypocenters determined with (a) the standard HYPOINVERSE program with flat-layered structure used by the USGS, (b) our new program QUAKE3D with flat-layered structure, and (c) QUAKE3D with dipping-layered structure.

transition we observe from a thin to a diffuse zone of seismicity. Previous work also proposed that the seismicity associated with the Mendocino transform fault dips steeply to the north, whereas our relocations indicate that it dips to the south. A small zone of intense seismicity just offshore of Cape Mendocino (Fig. 29) apparently is associated with the buckling of the southern edge of the Gorda plate against the thicker and more rigid Pacific plate. The seismicity is located beneath the Eel River basin near the point where the Mendocino Fracture Zone intersects the coastline. Future work will delineate the geometry and style of this deformation to determine how the fracture zone interacts with the San Andreas Fault System.

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Figure 29.
North-South cross
section of seismicity
(-124.8 to -124.5°)
using hypocenters
determined with
QUAKE3D with
dipping-layered
structure.

Investigations Using Large Array Teleseismic Data: Receiver Functions and Upper-Mantle Discontinuities

Principal Investigator: Paul Davis (UC Los Angeles)

LLNL Collaborator: George Zandt

Student: Philip Slack (UC Los Angeles)

Abstract

UC Los Angeles in conjunction with Los Alamos National Laboratory collected teleseismic data from a seismic array extending across the Rio Grande Rift from Winslow, Ariz. to Carlsbad, N. Mex. We used these data and the analysis expertise of LLNL personnel to study crustal structure and to search for upper-mantle discontinuities. Recent work using long-period data demonstrated the existence of upper-mantle discontinuity phases. Our goal is to look for these phases in short-period data using array-processing techniques. For a Northern Chile event we have identified the Pp400p phase and two arrivals that could be a Pp670p phase. With further analysis we hope to determine the depth and thickness of the 670-km discontinuity beneath the Rio Grande Rift.

Objectives

The objectives of our work are to investigate two approaches to analyzing teleseismic-array data. The first approach, begun in 1989, uses receiver functions to look at the structure of the crust and upper mantle beneath our array. The second, begun in 1990, uses array processing techniques to search for upper-mantle discontinuity phases in short-period data.

The receiver function technique provides a means to obtain structural information beneath a single three-component seismic station. A receiver function is the seismic response of the crust to an incident teleseismic plane wave with a single impulsive time function (i.e., a crustal Green's function). It is obtained by a deconvolution procedure applied to a three-component recording of a teleseismic *P* wave. The receiver function is then inverted for the crustal velocity function. Because our array spanned three geological provinces, our goal was to map this structure across the array from the Colorado Plateau over the Rio Grande Rift and onto the Great Plains.

The existence of discontinuity phases (arrivals that have reflected off the surface of the earth then off a discontinuity, such as the 670- or 400-km discontinuity) was demonstrated by Shearer when he stacked the Global Digital Seismic Network data.¹ These records were long-period records. We plan to look for these phases using our array of short-period data and array processing. Normally such phases would not be distinguishable in a short-period record, but with array processing we should be able to enhance the signal enough to make them visible. Our work differs from Shearer's in specific ways: we are using shorter-period data, which allows better resolution, and we are looking at paths over a specific geological region rather than at global averages.

Progress

Initial attempts to create receiver functions without correcting for instrument responses did not give good results. The vertical instruments used were Geotech S-13s with a 2-s center period, and the horizontal instruments were Kinemetrics SH-1s with a 5-s center period. The receiver functions with the calibrated data, although much improved, still contain too much pre-event noise to be reliable. The noise is of the same or greater magnitude than any signal arriving after the initial *P* wave. We must find ways to improve the signal-to-noise ratio if we are to use this technique.

Our first search for discontinuity phases indicates that we can find the $Pp400p$ arrival and two possible $Pp670p$ arrivals (Fig. 30). These discontinuity phases are consistent regardless of the number of stations used and can be enhanced with as few as four stations. They all have reversed polarity with respect to the P arrival, as expected for a discontinuity phase. The fact that we are seeing two possible $Pp670p$ arrivals still requires some explanation. The reflection at the 670-km discontinuity could be at either the source or receiver side of the ray path, so the two arrivals may indicate different depths to the 670-km discontinuity for the two possible paths. An alternative explanation is that the discontinuity is in two steps rather than one big discontinuity. Long-period data would not resolve this detail. More work will have to be done before we have a definite interpretation. We plan to analyze events from other azimuths and epicentral distances. First we will identify more of these phases, then we will investigate what we can learn about the deep structure of the receiver and source regions using this technique.

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Figure 30. Beamform for discontinuity phases. The uppermost trace is the low-pass filtered, stacked beam formed from the lower four traces for an event in Northern Chile. (The second from the top is the unfiltered stack.) The P wave pulses, filtered and unfiltered, are in the insert on the lower right. Arrival A is the 400-km discontinuity arrival, and arrivals C and D are the two possible 670-km discontinuity arrivals.

Broadband Wavefront Analysis of Rupture Processes of Large Earthquakes Along the Kermadec Subduction Zone

Principal Investigator: Heidi Houston (UC Santa Cruz)

LLNL Collaborator: Susan L. Beck

Abstract

We assessed the significance of the anomalous 1986 Kermadec earthquake for subduction-zone mechanics, the stress distribution along the Kermadec subduction zone, and the regional seismic potential. Our investigations indicate that faulting in the Kermadec earthquake occurred within the descending lithosphere rather than on the convergent plate boundary that is responsible for most large, shallow earthquakes in the region. Focal mechanisms obtained by inversions of surface waves and broadband body waves, and from first motions agree roughly and yield an oblique-compressional mechanism that does not fit easily into the regional tectonics. Relocation of the main-shock-aftershock sequence suggests that most of the aftershocks are not true aftershocks but represent triggered slip on the main thrust interface. The depth, relatively high stress drop, short duration of slip, and paucity of true aftershocks are consistent with intraplate faulting. Large intraplate events are rare, and almost all large, shallow, intraplate events in subduction zones exhibit downdip tension and can be attributed to slab pull. The Kermadec earthquake possesses neither downdip compression nor downdip tension, and is, therefore, virtually unique for its size. It may be related to lateral segmentation of the downgoing lithosphere.

Objectives

The Kermadec subduction zone (located in the southwestern Pacific Ocean, northeast of New Zealand) has been relatively neglected in the systematic study of subduction zones. Our objectives were to determine source parameters of the October 20, 1986 Kermadec earthquake moment magnitude ($M_w = 7.7$) and to consider their implications in the context of subduction-zone mechanics in the region. This earthquake, the second largest in 1986, is truly anomalous in its focal mechanism, stress drop, duration, and aftershock sequence. Understanding this event is therefore important for improving our knowledge of earthquake mechanics, subduction dynamics, and issues of resolution in surface and body wave inversions.

Progress

To characterize source parameters of the 1986 Kermadec earthquake at long periods, we performed an inversion of surface waves, in collaboration with visiting researcher Helen Anderson and postdoctoral researcher Jiajun Zhang (both of UC Santa Cruz).¹ The characterization included variation of the velocity and attenuation models assumed, the parametrization of the time function, and the set of Rayleigh waves included. The focal mechanism, seismic moment, centroid depth, and centroid time were quite stable with respect to these variations. The focal mechanism obtained ($\phi = 275^\circ$, $\delta = 60^\circ$, $\lambda = 158^\circ$) is similar to the Harvard group's solution. A seismic moment of 5×10^{27} dyn-cm and a centroid depth of 40 to 45 km were obtained. The focal mechanism and depth indicate that oblique slip occurred within the lithosphere in a very unusual orientation not on the plate boundary. The non-double-couple component of the moment tensor is less than 10%. Directivity of slip was poorly resolved. The centroid time of 10 to 13 s indicates an anomalously brief (by about a factor of two) duration of moment release for an event of this size.

The unusual long-period focal mechanism and the aftershock sequence, which includes many underthrusting events typical for the plate boundary along the Kermadec subduction zone but only two events with focal mechanisms similar to the main shock, raise the possibility that the main shock consisted of complex faulting corresponding to more than one focal mechanism. To assess the possibility of multiple focal mechanisms during the main shock, we continued our study of the broadband body wave forms of the Kermadec earthquake. They indicate a depth of about 35 km and some seismic slip (about 20% of the total) occurring 60 s after rupture initiation.² We used an iterative inversion that returns the best-fitting focal mechanisms for each iteration and the source time function. The focal mechanism returned by the first iteration for the slip that occurred from 0 to 15 s is roughly consistent with the long-period solution described above; later iterations become unstable. The mechanism of the slip at 60 s is as yet unresolved but appears to be different from the mechanism of the early slip. Multiple focal mechanisms during the first 20 s of moment release are not required or resolved, and the body waves appear to be adequately characterized by the long-period focal mechanism. We computed an average source spectrum from the teleseismic *P* waves and obtained estimates of the seismically radiated energy and the stress drop following results obtained by Houston.³ The energy is proportional to the area under the squared velocity spectrum, while the stress drop is obtained from the ratio of energy to moment. The estimated energy is 1×10^{23} erg and the stress drop (twice the apparent stress) is 30 bar. This stress drop is higher than similarly determined stress drops of interplate subduction earthquakes, and this is consistent with intraplate faulting with a relatively long repeat time rather than interplate faulting, which characteristically has a much shorter repeat time.

We relocated 60 aftershocks that occurred within three months of the main shock using the method of joint hypocentral determination (JHD), in collaboration with Susan Schwartz (UC Santa Cruz). Of 33 aftershocks with Harvard focal mechanisms, 26 have underthrusting mechanisms and shallow depths; only two have a mechanism similar to that of the main shock. The locations and mechanisms of the relocated aftershocks suggest that they are not true aftershocks. Rather, they represent triggered slip on the main underthrusting plate boundary (Fig. 31). Wave form modeling for the largest aftershock (December 21, 1986, $M_w = 6.2$) yields a depth of 17 km, consistent with the Harvard CMT depth. The main shock hypocenter appears to locate deeper than the main thrust interface on which the largest aftershock locates. This relation suggests that the main shock faulting occurred within the subducting plate, rather than at the plate boundary.

Figure 31. Cross-sectional view of relocated aftershocks of the 1986 Kermadec earthquake with focal mechanisms shown for the main shock (Oct. 20) and the largest aftershock (Dec. 21). Main shock faulting appears to have occurred within the subducting plate, rather than at the plate boundary.

Several factors suggest that slip in the main shock occurred along the roughly EW trending nodal plane, rather than along the roughly NS plane. First, there is a right-lateral offset in the free-air gravity anomaly perpendicular to the trench near the epicenter that would correspond to the right-lateral component of the slip associated with the EW nodal plane. Also, the strike of the trench changes near the epicenter: north of 28.36°S the trench strikes N10E; south of that latitude it strikes N20E. Furthermore, the relocated aftershocks are generally shallower in the northern part of the aftershock zone than in the southern part. These factors suggest that the subducting lithosphere may be segmented near the site of the Kermadec earthquake. Such lateral segmentation could be caused by the buoyant Louisville Ridge, which intersects the trench about 250 km to the north and may act as an obstacle to subduction.

The orientations of stress release determined from long-period surface waves, from the broadband body waves, and from first motions agree roughly and are consistent with oblique faulting within the plate that does not fit easily into the regional tectonic framework. The depth, short duration, relatively high stress drop, and paucity of true aftershocks also indicate intraplate faulting. An oblique-compressional event of this size within the shallow downgoing lithosphere is rare in a subduction-zone setting. The Kermadec earthquake may be associated with segmentation of the subducting plate.

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Seismological Investigation of Upper-Mantle Discontinuities Using Broadband Data

Principal Investigator: Susan Y. Schwartz (UC Santa Cruz)

LLNL Collaborator: Susan L. Beck

Abstract

We undertook a global and systematic analysis of broadband seismograms to characterize the variability in the existence, depth, and sharpness of upper-mantle discontinuities. We found that transversely polarized S waves make up the largest quantity of high-quality data to observe the presence and nature of upper-mantle reflected or converted phases. Stacking broadband seismograms from different earthquakes recorded at the same station and from different earthquakes recorded at stations in the same tectonic setting (e.g., the stable shield and platform of North America) does not reveal strong arrivals related to the upper-mantle discontinuities. However, low-pass filtering of the stacked SH wave forms results in arrivals produced by reflection or conversion at discontinuities in the upper mantle. This frequency dependence of reflected-wave amplitude can be exploited to obtain information on the sharpness of upper-mantle discontinuities.

Understanding the fate of subducted lithosphere, specifically whether it penetrates the 670-km discontinuity, can provide strong constraints on the nature of this seismic boundary. Slab penetration below the 670-km discontinuity would support the existence of a phase transition rather than a change in the chemical composition at this depth. We examined shear-wave travel times, amplitudes, and broadband wave-forms from events in the Kuril slab to place constraints on the velocity heterogeneity and on the depth of penetration of the subducted oceanic lithosphere. We found that slab heterogeneity is less pronounced for S waves than would be expected from previous P-wave studies. Our shear wave data do not require slab penetration into the lower mantle.

Objectives

Nearly all published models of seismic velocities contain abrupt velocity increases in the upper mantle at depths near 400 and 670 km. These seismic discontinuities indicate that phase changes or changes in chemical composition occur at these depths. Whether a phase change, compositional change, or both occur at the discontinuities is unresolved. Determination of the nature of the discontinuities is important for understanding the dynamics of mantle convection. Seismological data can help to constrain petrologic models of the seismic discontinuities. Our goal is to characterize these discontinuities, in particular their depth and sharpness, and to evaluate whether subducted slabs can penetrate the 670-km discontinuity.

Progress

We have made an extensive collection and examination of broadband digital wave forms oriented to generate reflected or converted phases from upper-mantle discontinuities.^{1,2} Our intent was to concentrate on S-to-P converted waves generated at the 670-km discontinuity, but too few seismograms with high signal-to-noise ratio existed to carry out a global characterization of the 670-km discontinuity using

these converted phases. Transversely polarized shear waves, recorded at station distances favorable to the generation of topside reflected phases $S400S$ and $Ss670s$ and bottomside reflected phases $S400S$ and $S670S$ (Fig. 32) from the 400- and 670-km discontinuities, were numerous and of exceptionally high quality to replace the Sp phase in our global characterization of upper-mantle discontinuities.

We have identified over 50 well-distributed events with strong SH radiation and excellent signal-to-noise characteristics to analyze upper-mantle reflected phases. We have stacked these broadband seismograms to enhance the visibility of the weak seismic signal expected from upper-mantle reflected phases. To establish the regional characteristics of the 400- and 670-km discontinuities, we have stacked data from different earthquakes recorded by a common station or by stations located in the same tectonic province. Our result is that broadband stacks show little evidence of upper-mantle converted phases. However, upon low-pass filtering, arrivals with travel times corresponding to upper-mantle reflected phases are visible. Figure 32 shows stacked data aligned on the Ss phase for shallow events recorded at the Regional Seismic Test Network stations within the stable shield and platform regions of North America. This stack reveals no obvious arrivals corresponding to the expected arrival times of the upper-mantle reflected phases (marked in Fig. 33). However, when this stack is low-passed filtered with a corner frequency of 0.067 Hz (~ 15 s), arrivals having approximately the predicted arrival times of the $S670S$ and $S400S$ phases are apparent. A frequency dependence to SH reflected wave amplitude is suggested by the absence of strong upper-mantle reflected arrivals on the broadband stacks and by their presence in longer period stacks. This frequency dependence is important and requires further study.

Figure 32. S -wave topside ($Ss400s$ and $Ss670s$) and bottomside ($S400S$ and $S670S$) reflections from seismic discontinuities at 400 and 670 km.

Our search for the effects of a deep slab extension of the Kuril slab reveals: wave form complexity for broadband S waves is not systematically organized with respect to postulated deep slab structure; a combination of deep-mantle and near-receiver structure can explain most of the S wave travel time patterns; S and ScS amplitude and travel-time patterns are not well correlated, but, ScS/S amplitude ratios and $ScS-S$ differential travel times show a rather high positive correlation. These findings strongly indicate that slab heterogeneity is less pronounced for S waves than would be expected assuming slab geometries derived from previous P -wave studies. This work supports several recent analyses of P waves that indicate that near-source and lower-mantle slab heterogeneity may have been overpredicted, and that slabs may not penetrate below the 670-km discontinuity.

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Figure 33. Broadband (top) and filtered (bottom) SS stacks. Markers T1, T2, T3, and T4 indicate the arrival times of the S, S670S, S400S, and SS arrivals. Note that the bottomside reflections are more clearly observed on the filtered stack.

Constraints on Early Mantle Segregation Processes and Komatiite Phase Equilibria

Principal Investigator: Quentin Williams (UC Santa Cruz)

LLNL Collaborator: Frederick Ryerson

Student: Daniel Farber (UC Santa Cruz)

Abstract

The compositions of major upper-mantle minerals, olivine and garnet, were examined in equilibria with highly magnesian silicate liquids at pressures up to 8 GPa. Such liquids have been inferred to exist within the early Earth's deep interior following the accretion of the planet. Their cooling and solidification is likely to have dominated the early chemical stratification of the Earth. These results therefore provide fundamental constraints on the development and composition of mantle geochemical reservoirs, the degree of stratification of the Archean mantle, and the structural properties of silicate melts relative to their coexisting solids at high pressure.

Objectives

Our goal has been to use the LLNL cubic multianvil press for experiments on element partitioning between silicate melts and their coexisting solids at high pressures and temperatures. The critical question is the degree to which the present composition of the Earth's upper mantle was affected by a process which occurred in the first 10 to 100 million years of the Earth's history. During this early period, it is plausible that the Earth melted to a depth of at least 600 km. Our studies have therefore focused on the partitioning behavior of transition metal elements, such as iron and nickel, and on widely used geochemical tracers, such as scandium and tantalum.

Progress

The Livermore large-volume press was calibrated in 1990 to pressures in excess of 18 GPa using the standard fixed-point pressure scale: in particular, calibration runs were based on discontinuities in the conductivities of Bi, ZnS, and ZnSe at 300 K. To characterize the effect of high temperatures on the pressure within the cell at constant load, the coesite-stishovite transition is being investigated under several high-pressure/high-temperature conditions. We estimate our ability to measure pressure and temperature in these experiments as being ± 0.5 GPa at temperatures in excess of 2000 K.

Following calibration of the instrument, a number of large-volume press runs were conducted on melts formed by partial fusion of komatiitic starting materials at pressures of 8 GPa and above. Consistent with lower-pressure partitioning studies, we observe significant enrichment of iron in the melt relative to that within the solid assemblage at these pressures. As a result, not only does the melt become denser at high pressures, but iron partitioning into the liquid generates the anomalous negative buoyancy of olivine crystals in ultrabasic melts at high pressure. These data,

combined with silicate melt equation of state parameters, provide fundamental constraints on the magnitude of different effects in giving rise to buoyant crystals within a deep terrestrial magma ocean. Our results also indicate that the difference in temperature between liquidus and solidus in komatiitic liquids is only 100 to 200 K in this pressure range. Therefore, the solidification of a deep magma reservoir of komatiitic composition is likely to proceed over a fairly narrow temperature range.

The textures produced in our preliminary experiments indicate that the current configuration may be quite useful for the determination of mineral-melt partitioning in spite of large thermal gradients. The gradient drives thermal migration, resulting in a melt-free crystalline assemblage at the cold ends of the sample and crystal-free melt in the center (Fig. 34). Microprobe analysis indicates that the melt is homogeneous, allowing broad-beam analysis to be employed. Mineral-melt partition coefficients can be obtained by analyzing the solid phases at the interface.

Figure 34. Backscattered electron image of a sample quenched from 1700°C, 45 kbar. The mineral phase olivine (Ol), garnet (Gt), and clinopyroxene (Cpx) present at both ends of the sample are separated by a pool of melt (M) represented by a mat of quench crystals. The melt-solid interface represents an isotherm.

A Stable-Isotope Study of Groundwater Migration in the Eastern Livermore Valley

Principal Investigator: Lewis Cohen (UC Riverside)

LLNL Collaborators: Richard Thorpe and David Rhee

Student: G. Richard Rees (UC Riverside)

Abstract

Stable isotopes of oxygen and hydrogen were used to characterize groundwater migration in the eastern Livermore Valley. Analyses of well waters from the LLNL vicinity have detected a region of isotopically light water located in the southwest portion of LLNL. Isotopic variations with depth and time are being monitored within the anomalous region. The results of this study will aid investigations of contaminant migration in the groundwater near LLNL.

Objectives

Water from several test wells at LLNL showed that an isotopic anomaly (in both hydrogen and oxygen isotopes) exists in the groundwater under the site. The isotopically light water responsible for the anomaly may derive from one or more of the following: a recharge ten years ago with Sierra Nevada water from the South Bay Aqueduct (SBA) by the local water agency, leakage from the SBA near LLNL, or leakage from water lines and sewer pipes of Hetch Hetchy (imported high Sierra) water used for most purposes at LLNL. Our objective was to identify the extent of the anomaly and use the data to obtain new information on the rates and mechanisms of groundwater migration near the Laboratory. Muir and Coplen¹ performed

Figure 35. δD vs $\delta^{18}O$ for groundwater and SBA, and average global precipitation (represented by the meteoric water line). The approximate measurement of the error boxes is 2σ . Waters from 7D2 and MW-318 show partial evaporation. Although showing seasonal fluctuations, SBA water falls on the meteoric line. Waters from wells within the isotopic anomaly fall between the isotopic end members along a line of mixing approximated by the meteoric water line. Points which fall off the meteoric water line probably represent errors in analysis or sampling or a significant contribution of waters partially evaporated in the vadose zone.

a similar study involving recharge water from the SBA in the Santa Clara Valley. However, their work was limited by a paucity of wells in the region of recharge. The abundance of monitor wells at LLNL (over 250 in one square mile) and the frequency with which these wells are monitored provides a rare opportunity to study groundwater migration with stable isotopes. This study also will provide general information on groundwater flow in inhomogeneous fluvial sediments, which may be useful in groundwater studies in areas with similar geology.

Analyses of 68 samples for D/H and 23 for $^{18}\text{O}/^{16}\text{O}$ were completed on the VG mass spectrometer at UC Riverside. Figure 35 shows the range of isotopic values relative to the SMOW isotopic standard. The local groundwater is in the range of δD -45 to -50‰ (‰ = per mil) with a component of vadose zone evaporation in near surface waters. SBA water falls on the meteoric water line with a seasonal fluctuation ranging from -72 to -74‰. Groundwater from wells at LLNL lies on a mixing line (approximately the meteoric water line) between the two extreme values. Waters that fall off the meteoric water line may have a component of water partially evaporated in the vadose zone.

Figure 36 shows the δD values for the distribution of near-surface groundwater. The anomaly is distributed bilaterally around the Arroyo Seco drainage with the lightest water at the southwestern corner of the site. The pattern in Fig. 36 suggests a light-water source near the Arroyo. However, no simple mechanism for easterly flow of light source water near the Arroyo exists because present and historic groundwater flow is generally westward.²

Progress

Figure 36. Wells sampled and δD values for shallow groundwater at LLNL. The anomaly is centered around the Arroyo Seco. The light isotopic value in the northwestern portion of LLNL (MW-5) may result from leakage from a 27-in. SBA distribution line, which runs along the northern boundary of LLNL. Groundwater flow directions are from Dresen and Hoffman.²

Analyses on nests of wells of different depths indicate that the anomaly is variable in thickness. The thickness is greatest in the southwest and decreases toward the east. One well nest west of the site shows the anomaly as a distinct layer of light water bounded above and below by heavier water. This suggests at least one cycle of alternating local and imported water sources.

A few wells have been tested for a change in stable isotope values over time. The maximum time between sampling was eight months, and no significant change was observed.

To further constrain and define the areal extent of the isotopic anomaly, a number of the local water agency's wells and private wells outside the general vicinity of LLNL will be analyzed. Additional isotopic analyses will test our hypotheses of groundwater movement in the eastern Livermore Valley. Data obtained in this study will be used as input in the computer groundwater model SLAEM to identify the flow rates near LLNL.

The isotopic data already obtained will help solve practical problems related to the LLNL Environmental Restoration Program. One problem is the extent of replacement of local water in pore fluids by drilling fluid during well construction. Future work will include isotopic comparisons of pore fluids from well corings in the saturated zone with drilling fluids (Hetch Hetchy water). This will help determine how accurately core pore fluids (tested for volatile organic compounds) represent actual pore fluids.

References

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2. Dresen, M. and Hoffman, F., 1986, *Volatile Organic Compounds in Ground Water: West of LLNL: Lawrence Livermore National Laboratory Site and Adjacent Areas*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-53740.

Biogeochemical Cycling of Trace Metals in the California Offshore Environment by ICP-Mass Spectrometry: The Impact of the *Pacbaroness* Shipwreck

Principal Investigator: Stanley V. Margolis (UC Davis)

LLNL Collaborator: G. Price Russ III

Student: Philippe Claeys (UC Davis)

Abstract

Maritime disasters are an increasing threat to the environment. An example is the sinking of the 564-ft freighter Pacbaroness on September 27, 1987 in 430 m of water, after a collision with another freighter in fog off Point Conception, Calif. Two research cruises were conducted at the site within four months of the sinking to determine the effect of its cargo—23,000 tons of powdered copper ore and 400,000 gal of fuel oil—on the marine environment. This productive and unique area includes several commercial fisheries and the Channel Islands National Marine Sanctuary. Both dissolved copper and fuel oil are toxic to a variety of marine organisms. Preliminary studies indicated that the diversity and abundance of benthic organisms were severely reduced within a 500-m radius of the wreck, where the copper ore and fuel oil were concentrated. We also have refined ICP-MS techniques for analyzing trace elements in marine sediments and marine organic tissues. In addition, we found that several chemical elements from the spilled copper ore, including Cu, Ag, Sb, As, Cd, Mo, Zn, and Se, made their way into the sediments and marine organisms in the immediate area of the wreck.

Objectives

Our goal is to evaluate the long-term environmental effect of the *Pacbaroness* shipwreck on the regional benthic ecosystems. We will conduct time-series sampling and analyses of copper, other toxic trace metals, and hydrocarbons in sediments, seawater, and marine organisms from the area around the wreck. We will determine whether the contamination is a persistent threat to water quality, commercial fisheries, and Channel Island National Marine Sanctuary by comparing data collected four months after the sinking with data collected three to five years later. If these resources are threatened, this study will facilitate the formulation of a cleanup/mitigation plan to reduce the long-term environmental damage in this area.

This study, the first of its kind in deep (430-m) waters, will be valuable in assessing the potential environmental impact of future spills on the continental shelf and slope. Our study also will be of great importance to policymakers interested in preventing future marine disasters and to scientists interested in sediment and pollutant transport processes, marine benthic ecology, marine toxicology, and biogeochemical mechanisms.

Progress

Preliminary ICP-MS analyses (Fig. 37) indicate that trace metals (Cu, Ag, Sb, As, Cd, Mo, Zn, Pb, and Se) found concentrated in the ore were also found concentrated in the upper 10 cm of the sediment. The same elements were found in the tissues of sea urchins, suggesting that this technique provides an excellent means of tracing the pathways of these metals through the marine biogeochemical cycle. Analyses of internal organs from the sea urchins showed progressive trends of enrichment in specific trace elements in their digestive and reproductive systems.

Similar analyses of the livers from Dover sole and rockfish, two commercial species from the California Shelf, indicated that there was no appreciable bio-accumulation of copper four months after the copper ore spill. The ICP-MS analyses, however, indicate that several other metals enriched in the ore were found at sublethal, but elevated, concentrations in site fish, in comparison with the control station. Differences in mobility, range, and feeding strategy can explain the delay in accumulation of these trace elements.

Figure 37. Copper and metal content of sediment (ppm) shown with station locations around the Pacbaroness shipwreck off Point Conception, Calif.

Ideal Body Analysis of the NTS Tower Experiment

Principal Investigator: Mark A. Zumberge (UC San Diego)

LLNL Collaborator: Paul W. Kasameyer

Abstract

Experiments that rely on potential theory alone to test the validity of Newton's inverse square law of gravity, a subject of current debate, are imperfect because of practical sampling limits. We developed a test that finds the smallest underground density contrast consistent with a set of gravity observations. Recently, we used this test to show that none of the recent geophysical experiments showing anomalous vertical gravity gradients provides compelling evidence for a breakdown of Newton's law. We apply this methodology to the experiment being performed by an LLNL group on a tower at the Nevada Test Site. Using gravity ideal bodies, we determine how well a given ground survey constrains the vertical gravity gradient subject to an acceptable underground density contrast. This allows us to assess the ability of the experiment's geometry to test the validity of the inverse-square law. We also will evaluate the relative merits of the ideal body approach compared with the traditional potential integral.

Objective

Experiments have been performed to test the validity of Newton's inverse-square law of gravity. Several of them, including one carried out by an LLNL group, compared values of gravity measured on a tall tower with values predicted using Newtonian theory. We proposed to analyze their experiment using gravity ideal bodies.

Progress

The LLNL group, which includes John Thomas, Paul Kasameyer, and Orrin Fackler, used measurements along the BREN Tower at the Nevada Test Site (NTS). Kasameyer provided the locations at which surface gravity was observed. We have not received the actual values of gravity observed at those locations (we understand that additional values are still being obtained).

We began our analysis by forming ideal bodies of varying density that are consistent with values of zero for the surface gravity anomalies and with gravity values along the tower governed by an artificial slope. The point of this analysis is twofold. First, we want to explore the number and coarseness of cells in the ideal body space that are needed to adequately perform the inversion. Second, even without having the actual gravity data, we can assess the uncertainties in upward-continued values of gravity by varying the artificial slope until the pseudo-data can no longer be fitted with a reasonable density contrast in the ideal body.

Our conclusions are limited by the computational abilities of the machine on which we have been working. Our largest inversion fitted 358 points with a body having 4000 cells. This required several hours on a Sun 4. To adequately fit the data, we plan to perform a larger inversion on a Cray YMP (20 hr of Cray time were allotted to us as part of the award).

The inversions on the Cray will begin in coming months. We also have requested the complete data set from the LLNL group. Without the actual gravity values at the observation points, our study will simply be a different way to calculate uncertainties in the upward continuation based on the distribution of the ground points.

Section IV. IGPP-LLNL Workshops and Seminars

Center for High-Pressure Sciences

Workshop

Iron Workers Convention Update

A workshop called the Iron Workers Convention was held in June, 1989 at Los Alamos National Laboratory. It was sponsored jointly by IGPP branches at Los Alamos, UC Los Angeles, and Livermore. The purpose was to discuss the state of knowledge of Fe at the high pressures and temperatures in the core of the Earth and directions of future research to elucidate the nature of the Earth's core. Thirteen papers presented at the workshop have since been published in a special section of the *Journal of Geophysical Research* (*J. Geophys. Res.* **95** (B13) 21 587-21 767 (1990)).

Seminars

October 5, 1989

"Pressure Induced Resonant Raman Scattering in Semiconductors"

A. Jayaraman, Bell Laboratories

October 31, 1989

"Determining Nuclear Yield for Treaty Verification"

William Moss, Earth Sciences, LLNL

November 16, 1989

"High Pressure Supercritical Fluids: Thermophysical Properties, Phase Equilibria and Combustion"

E. Ulrich Franck, University of Karlsruhe

November 20, 1989

"Dynamic Compression and Release Studies of Geologic Materials"

Michael Furnish, Sandia National Laboratories, Albuquerque, NM

December 4, 1989

"Shock Synthesis of Wurtzite-Phase Boron Nitride"

Mastada Araki, Chemicals & Explosives Laboratory, Japan

December 18, 1989

"Sm-YAG: A Pressure Calibrant for High Temperature and Pressures"

Nancy Hess, University of Washington

December 19, 1989

"Electronic Attraction in Condensed Matter"

Neil Ashcroft, Cornell University

January 4, 1990

"Current Issues in Static High Pressure"

Sergei Stishov, Institute of Crystallography, Moscow, and Cal Tech

January 5, 1990

"Pressure and Magnetic Studies of Electron Doped CuO Superconductors"

John Markert, University of California, San Diego

January 25, 1990

"Polarized Targets for Hydrogen Fusion"

Clark Souers, Chemical Sciences Division, LLNL

February 1, 1990

"Predicting Properties of Solids, Clusters, and Superconductors"

Marvin Cohen, University of California, Berkeley

March 29, 1990

"Shock Compression of Solids: a Tutorial"

William Nellis, H-Division/IGPP, LLNL

March 30, 1990

"Recent Transport Measurements in High- T_c Superconducting Oxides"

Alex Zettl, University of California, Berkeley

April 5, 1990

"Chemical Equilibrium? Models of Transient States: Foams and Carbon"

Mat van Thiel, H Division, LLNL

April 26, 1990

"Strong Correlation in the Cuprates"

Andy McMahan, H Division, LLNL

May 18, 1990

"Phase Behavior of Binary Mixtures at High Pressure: Experiments and Theoretical Calculations"

Willem L. Vos, Universiteit van Amsterdam

May 31, 1990

"Studies of High Temperature Superconductors and High Pressure Hydrogen"

Troy Barbee III, University of California, Berkeley

June 18, 1990

"Optical Properties of High-Pressure Nonideal Plasmas"

Vladimir Fortov, High Temperature Institute, Moscow

June 18, 1990

"Computer Simulations of Detonation Phenomena"

Tatiana Fortova, Institute of Chemical Physics, Chernogolovka, USSR

June 19, 1990

"Non-additive Interactions in Simple Molecular Crystals and Interaction of Picosecond Laser Pulses with Metals"

Sergey Anisimov, Landau Institute of Theoretical Physics, Moscow, USSR

June 28, 1990

"Liquid Carbon"

Richard M. Martin, University of Illinois

July 2, 1990

"Plasmas Produced by the Shock Compression of Gases"

G. I. Mishin, Ioffe Physical-Technical Institute, Leningrad, USSR

July 2, 1991

"Theory at High Temperature Superconductivity"

Alexei A. Abrikosov, Institute of High Pressure Physics, Moscow, USSR

July 3, 1990

"Recent Results in Static High Pressure Research"

S. M. Stishov, Institute of Crystallography, Moscow, USSR

July 11, 1990

"Hot Forging: A New Method to Densify SHS-Produced TiC"

Lothar W. Meyer, Fraunhofer Institute for Applied Research of Materials,
West Germany

Astrophysics Research Center

Seminars

October 10, 1989

"Hot-CNO Cycle and the RP-Process Nuclear Reactions"

Shigeru Kubono, University of Tokyo

October 13, 1989

"Stellar Winds"

Frank Pijpers, University of Leiden, Netherlands

October 17, 1989

"Particle Acceleration Mechanisms in Ultra-high Energy Gamma-ray Sources"

Alice Harding, NASA, GSFC

October 20, 1989

"Measuring the Geometry of the Universe"

Ed Loh, Michigan State University

October 27, 1989

"Low-Mass Brown Dwarfs in Taurus"

William J. Forrest, University of Rochester

November 3, 1989

"s-r-Process Evolution in the Galactic Halo and Disk"

Grant Bazan, IGPP, LLNL, and the University of Illinois

November 10, 1989

"The Ratio of Hydrogen to Helium in Globular Clusters"

George Wallerstein, University of Washington

November 17, 1989
"High Redshift Galaxies"
Ruth Daly, Princeton University

November 22, 1989
"Gamma-Ray Observatory"
Dieter Hartmann, LLNL and Stanford University

December 1, 1989
"The Pulsar in SN1987a"
Robert V. Wagoner, Stanford University

December 8, 1989
"Nuclear Synthesis of Neutron Capture Elements in the Early Galaxy"
Chris Sneden, University of Texas

December 13, 1989
"Neutrinos as Dark Matter in the Singlet Majoron Model"
Eric Carlson, Lawrence Berkeley Laboratory

December 15, 1989
"Shadows of Creation"
David N. Schramm, University of Chicago

January 5, 1990
"Chemodynamical Evolution of the Galaxies"
Andy Burkhard, University of Illinois

January 12, 1990
"Black Holes, the QCD Phase Transition, and Nucleosynthesis"
Eric Carlson, Lawrence Berkeley Laboratory

January 19, 1990
"Lithium in AGB Stars"
Vern Smith, University of Texas

January 26, 1990
"Compton Scattering in Strong Magnetic Fields and the Continuum Spectra of Gamma-ray Bursts"
Chuck Dermer, LLNL and Space Science Laboratory, Berkeley

February 2, 1990
"Mapping of the Universe"
Margaret Geller, Harvard Smithsonian, Center for Astrophysics

February 15, 1990
"Model for Active Galactic Nuclei"
Amri Wendell, Weizmann Institute, Israel

February 16, 1990
"Quarks in the Early Universe"
Craig Hogan, University of Arizona

February 23, 1990

"The Decline and Fall of Classical Novae"

James Truran, University of Illinois

March 9, 1990

"Instabilities Mixing and Clumping in SN 1987A"

Bruce Fryxell, University of Arizona

March 12, 1990

"Is There a Primordial R-Process?"

R. K. Thielemann, Harvard Smithsonian Center for Astrophysics

March 16, 1990

"Domain Walls in the Early Universe"

Larry Kawano, California Institute of Technology

March 23, 1990

"Periodicity in the Large Scale Distribution of Galaxies"

David Koo, University of California, Santa Cruz

March 26, 1990

"Relativistic Shocks in Pulsar Winds"

Jonathan Arons, University of California, Berkeley

March 30, 1990

"Recent Results of Coded Aperture Gamma Ray Observations of the Galactic Center and SN 1987A"

Tom Prince, California Institute of Technology

April 5, 1990

"Mixing in SN 1987A"

Ken Nomoto, University of Tokyo

April 6, 1990

"Galactic Chemical Evolution"

Grant Bazan, University of Illinois

April 18, 1990

"The Spectrum and Intensity of the Cosmic X-Ray Background"

Xiaoyi Wu, Columbia University

April 20, 1990

"Extended Inflation"

E. W. Kolb, Fermilab and University of Illinois

April 23, 1990

"Accretion-Powered White-Dwarf Pulsars"

Joseph Patterson, Columbia and University of California, Los Angeles

April 25, 1990

"Evolution of Pulsars: Our Most Accurate Clocks"

Roger Romani, Institute for Advanced Study

April 27, 1990

"High Resolution Optical Absorption Studies of the Local Interstellar Medium"

Barry Y. Welsh, Space Sciences Laboratory, University of California, Berkeley

May 4, 1990

"A New Model for 10^{15} eV Gamma Ray Sources"

Ian Smith, Washington University at St. Louis

May 9, 1990

"Gamma Rays from Neutron Stars"

Malvin Ruderman, Columbia University

May 11, 1990

"Equation of State for Neutron Stars"

William Meyers, Lawrence Berkeley Laboratory

May 11, 1990

"Evolution Statistics and Birthrates of Pulsars"

Jeremiah Ostriker, Princeton University

May 14, 1990

"Simulation of Bounded Multiscale Plasmas"

Scott Parker, University of California, Berkeley

May 18, 1990

"Q Stars"

Safi Bahcall, Stanford Linear Accelerator Center

May 25, 1990

"Physics on the Edge: Brown Dwarfs and Low Mass Stars"

Adam Burrows, University of Arizona

June 1, 1990

"Modeling the Dynamics of the Interstellar Medium"

Eric Keto, IGPP-LLNL

June 8, 1990

"Neutrinos in the Early Universe"

Robert Malaney, IGPP-LLNL

June 22, 1990

"High Temperature Neutrino Interaction Stellar Collapse"

Bradley S. Meyer, IGPP-LLNL

July 6, 1990

"Chaos in the Mixmaster Universe: The Real Story"

Beverly K. Berger, Oakland University, MI

July 13, 1990

"Pre-Main-Sequence Lithium Burning in the Hyades and the Sun"

Fritz Svensson, University of California, Santa Cruz

July 20, 1990

"New Astrophysical Opacities"

Forrest Rogers and Carlos Iglesias, LLNL

July 27, 1990

"Direct Reaction Mechanisms at Thermonuclear Energies"

H. Oberhummer, Vienna, Austria

August 3, 1990

"Primordial Black Holes"

Lawrence Hall, Lawrence Berkeley Laboratory

August 24, 1990

"Damped Lyman α Absorption Systems: Progenitors of Galactic Disks"

Art Wolfe, University of California, San Diego

September 14, 1990

"Evolution of Quasars and Radio Galaxies"

Vijay Kapahi, TATA Institute for Fundamental Research, India

September 21, 1990

"Star Formation, Structure and Kinematics of Molecular Clouds"

John Bally, Bell Laboratories, New Jersey

September 28, 1990

"The Search for Supermassive Black Holes"

Andrew Wilson, University of Maryland

Center for Geosciences

Workshop

The 84th Annual Meeting of the Seismological Society of America, May 2-4, 1990, Santa Cruz, Calif., cosponsored by IGPP-LLNL and UC Santa Cruz.

Seminars

November 29, 1989

"Early Thermal State of the Earth"

Michael J. Drake, University of Arizona

December 21, 1989

"New Results on the Thermodynamic Properties of Uranium in High Temperature Aqueous Solutions"

Dr. Igor L. Khodakovskiy, Vernadskiy Institute of Geochemistry and Analytical Chemistry, Academy of Sciences of the USSR, Moscow

January 23, 1990

"Cenozoic Plate Tectonics of the Northeastern Pacific and Western North America: New Developments"

Tanya Atwater, University of California, Santa Barbara

February 1, 1990

"Microscale Chemical Heterogeneity of Groundwater"

Mordecai Margaritz, Cal Tech

February 8, 1990

"Hydrodynamic Interaction in Colloidal Dispersions and Porous Media, Via Lattice-Gas Models of the Fluid Phase"

Tony Ladd, Earth Sciences, LLNL

February 15, 1990

"A Simple and Convenient Isotropic Failure Surface"

M. B. Rubin, Earth Sciences, LLNL

April 5, 1990

"Rupture Nucleation on Unfavorably Oriented Faults"

Richard Sibson, University of California, Santa Barbara

May 3, 1990

"Episodic Yoyo Movements (Epeirogeny) on Continental Platform and Intra-Cratonic Basins: Need for Reinterpretation of Paleogeography, Faunal Extinctions, and Source Rock Maturity"

Gerald M. Friedman, Rensselaer Center of Applied Geology

May 17, 1990

"Solution-Mineral Equilibria in Icelandic Geothermal Systems"

Stevan Amorsson, University of Iceland and Stanford University

May 23, 1990

"Nontraditional Petroleum Reservoir Mechanisms"

Michael Prats, University of Texas

May 24, 1990

"Chemical and Biological Degradation of Halogenated Solvents"

Timothy Vogel, University of Michigan

July 18, 1990

"Regional Modeling of Groundwater Flow in Fractured Rock Aquifers: Discrete Flow Modeling with Analytic Elements"

Stephen R. Kraemer, University of Virginia

July 26, 1990

"Behavior of Radionuclides at the Chernobyl Incident"

Igor L. Khodakovskiy, Vernadskiy Institute of Geochemistry, USSR Academy of Sciences, Moscow, USSR

September 4, 1990

"Electromagnetic Exploration of the Earth's Crust"

Gerhard Schwarz, Freie Universität Berlin, West Germany

Section V. Bibliography

1990

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Section VI. Fiscal Year 1991 IGPP-LLNL University Collaborative Research Program Awards

Principal investigators	Title
Kerridge (UCLA), Phinney (LLNL)	Ion microprobe analysis of amino acids in meteorites
Harrison (UCLA), Ryerson (LLNL)	Monazite as a thermochronometer for prograde metamorphism
Wolfenstine (UCI), Beeman (LLNL)	The effects of impurities on the creep behavior of NaCl following stress changes
Staudigel (UCSD), tenBrink (LLNL)	Alteration of mid-ocean ridge basalt glasses: mobility of trace elements and radionuclides
Lea (UCSB), Russ (LLNL)	Trace metals in stromatolites as a probe of climate change
Williams (UCSC), Ryerson (LLNL)	High pressure element partitioning and diffusion rates in ultrabasic melts
Flegel (UCSC), Niemayer (LLNL)	Determination of sources and fluxes in sediments from the Great Lakes
Elders (UCR), Proctor (LLNL)	Application of AMS to dating the younger sedimentary record of Lake Baikal, USSR
Lange (UCB), Labov (LLNL)	Superconducting tunnel junction for astrophysical research
Becker (UCD), van Bruegel (LLNL)	Studies based on a new catalog of 53,522 5-GHz sources
Morris (UCLA), Alcock (LLNL)	A numerical investigation of the stability of the gas-dust outflows from cool red giant stars
Gwinn (UCSB), Ball (LLNL)	10 micron infrared array imaging of W49N
Spinrad (UCB), van Bruegel (LLNL)	Optical properties of nearby radio galaxies
Fuller (UCSD), Mathews (LLNL)	The evolution of primordial baryon number fluctuations and Big Bang nucleosynthesis
Kahn (UCB), Hailey (LLNL)	Development of an imaging germanium drift chamber for gamma ray astronomy
Arons (UCB), Langdon (LLNL)	Relativistic shock waves in synchrotron sources

Principal investigators	Title
Flatte (UCSC), Max (LLNL)	Atmospheric characterization for adaptive optics
Schubert (UCLA), Carrigan (LLNL)	The influence of multiphase and multifluid effects on magma storage and transport processes
Berger (UCSD), Smith (LLNL)	Spectra and polarization of Lg observed at IRIS/IDA stations in the USSR
Archuleta (UCSB), Jarpe (LLNL)	Analysis of the site response of weak and strong ground motion from Coalinga, CA and Treasure Island, CA
Davis (UCLA), Zandt (LLNL)	Investigation of upper mantle discontinuities using large array teleseismic data
Houston (UCSC), Zandt (LLNL)	Seismicity and tectonics of Northern California
Wenk (UCB), Durham (LLNL)	Experimental deformation of ice: ductile flow and texture development
Shelton (UCD), Radousky (LLNL)	High temperature superconducting ($\text{Ba}_{1-x}\text{K}_x$) BiO_3 under extreme pressures
Fong (UCD), Mailiot (LLNL)	Realistic theoretical simulation of temperature-pressure quenching
Bukowinski (UCB), Boercker (LLNL)	Effects of pressure on viscosity of ionic liquids
Constable (UCSD), Duba (LLNL)	Electrical conductivity of mantle rocks to 1500°C
Alivisatos (UCB), Tobin (LLNL)	High pressure studies of semiconductor clusters
Nicol (UCLA), Yoo (LLNL)	Melting, other phase transitions and reactions of simple solids at high pressures
Maple (UCSD), Nellis (LLNL)	Dynamic high pressures synthesis of high T_c superconductors
Jeanloz (UCB), Akella (LLNL)	Ultra high pressure melting curve of uranium
Anderson (UCLA), Erskine (LLNL)	A new apparatus for measuring the thermal expansivity of minerals at high temperature