UCRL--53809

DE87 014618

**Institute of Geophysics
and Planetary Physics at
Lawrence Livermore
National Laboratory**

1986 Annual Report

Claire E. Max, editor
Manuscript date: July 1, 1987

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

MASTER

DISTRIBUTION OF THIS REPORT IS UNLIMITED

Acknowledgments

This report was edited, designed, and produced by Kevin Anderson. Most of the artwork was done by John Zych.

Table of Contents

	Introduction
IGPP Goals and Organization	1
Highlights of the 1986 Fiscal Year at the IGPP-LLNL	4
Seismic Wave Propagation and Structure of the Basin and Range, Nevada <i>J.S. McClain, with H. Patton, Y. Dilek, K. Priestly, and D. Chávez</i>	11
Simultaneous Hypocenter-Structure Inversions for the Santa Barbara Channel Region <i>W.A. Prothero, Jr., with J. Scheimer, J. Taylor, and J. Eickemeyer</i>	14
Earthquake Magnitude Estimation from Initial Waveform Analysis <i>T.V. McEvilly, with H. Patton, J. Scheimer, K. Mayeda, and J.E. Scheiner</i>	16
Seismic Data Telemetry via Satellite Using Spread-Spectrum Technology <i>J. Berger, with J. Scheimer and N. Burr</i>	19
Seismological Studies of Core-Transition Zones <i>L. R. Johnson, with F.E. Followill and P. Cummins</i>	21
Q Structure Beneath the Mono Craters—Long Valley Region of Eastern California <i>W.A. Prothero, Jr., with J. Scheimer, and L.K. Steck</i>	25
Seismic Discrimination at Small Magnitudes Using RSTN Data <i>T. V. McEvilly, with A. Smith, S. Taylor, and R. Grose</i>	28
Study of Complex Rupture Patterns Along the Calaveras Fault Using Broadband Digital Seismogram Data <i>K.C. McNally, with J. Scheimer, G. Nelson, and E. Brown</i>	31
Determination of Crustal Structure at Long Valley from Teleseismic Converted Energy <i>W.A. Prothero, Jr., with G. Zandt and L.K. Steck</i>	33
Dynamic Response of Fully and Partially Fluid-Saturated Rocks <i>W. Goldsmith and M.M. Carroll, with B.P. Bonner, R.C.Y. Chin, A. Imam, and B. Revisn</i>	36

Table of Contents

	Ion Chromatographic Analysis of Ice Core Samples from Central Greenland <i>H. Craig, with R. Finkel</i>	38
	Study of Heat Flow in the Salton Sea Geothermal Area and Its Adjacent Fault Zones <i>T.C. Lee, with P.W. Kasameyer and Z. Yi</i>	40
Center for High-Pressure Physics	Emission Spectra from Simple Shocked Solids <i>M.F. Nicol, with N.C. Holmes, M.L. Johnson, and S. Johnson</i>	43
	Statistical Mechanics and Phase Equilibria of Ionic and Geophysical Systems at High Pressure <i>M.S.T. Bukowinski, with M. Ross and G.H. Wolf</i>	48
	Melting of Simple Solids at High Pressures <i>R. Boehler, with M. Ross, D.A. Young, Z. Chang-Sieng, and M.F. Nicol</i>	52
	Deformation-Enhanced Dissolution in Theory, Experi- ment, and Nature, Based on Microstructural Evidence <i>H.R. Wenk, with H.C. Heard and A. Meike</i>	56
	Conductivity of Mantle Rocks Between 20 and 600°C <i>S. Constable, with A. G. Duba</i>	58
	Measurement of the Hall Effect in Olivine at High Temperature <i>C-Y Wang, with A. G. Duba and L. Hirsch</i>	60
	Dynamic High-Pressure Processing and Synthesis of Novel Materials <i>M.B. Maple, with W.J. Nellis, J. Neumeier, and M. Torikachvili</i>	63
Astrophysics Research Center	Nuclear Astrophysics and Radiation Transport <i>S.E. Woosley, with T. Axelrod, R. Klein, T. Weaver, D. Hartmann, P. Pinto, and J. Arons</i>	67
	Gravitational Perturbations in Spiral and Elliptical Galaxies <i>L. Hernquist, with C.E. Max, D. Merritt, and P.J. Quinn</i>	69
	Laboratory Studies in X-Ray Transfer Physics Relevant to Cosmic Sources <i>S.M. Kahn, with R. Lee, R.W. Falcone, M. Hettrick, R. London, G. Kolbe, W. Craig, and J. Schachter</i>	73
	The Emission Lines from Quasars and Seyfert Galaxies <i>R.C. Puetter, with G. Fisher, S. Langer, and I. Krinsky</i>	77

Table of Contents

Dynamics and X-Ray Spectra of Inhomogeneous Young Supernova Remnants <i>C.F. McKee, with C.B. Tarter and C.J. Romanik</i>	80
Computer Study of the Turbulent Mixing of Scalars <i>C.H. Gibson, with R.M. Kerr, W.T. Ashurst, and A.R. Kerstein</i>	82
Plasma Astrophysics <i>J. Arons, with B.I. Cohen, R.I. Klein, A.B. Langdon, C.E. Max, D. Burnard, and A. Zachary</i>	85

Introduction

IGPP Goals and Organization

The purpose of the Institute of Geophysics and Planetary Physics (IGPP) at LLNL is to enrich the opportunities of University of California campus researchers by making available to them some of the Laboratory's unique facilities and expertise, and to broaden the scientific horizon of LLNL researchers by encouraging collaborative or interdisciplinary work with other UC scientists.

The IGPP continues to emphasize three fields of research—geoscience, astrophysics, and high-pressure physics—each administered by a corresponding IGPP Research Center. Each Research Center coordinates the mini-grant work in its field, and also works with the appropriate LLNL programs and departments, which frequently can provide supplementary funding and facilities for IGPP projects.

At the core of the IGPP program at Livermore is a group of research “mini-grants” open to scientists from all UC campuses, and funded by the UC Regents and the LLNL Director. Proposals are peer-reviewed in the spring of each year by a committee of scientists from UC campuses, LLNL programs, and outside universities. Typical funding ranges from \$5000–\$20,000, and is used for a variety of purposes, including support for visiting graduate and post-graduate researchers, high-energy-density experimental facilities for visiting faculty researchers, and supercomputing time at the LLNL National Magnetic Fusion Energy Computer Center.

Figures 1–3 give a statistical overview of the participants in the IGPP mini-grant program. About half of the campus participation is from UC Berkeley; the remainder is distributed over six other campuses. A typical mini-grant consists of a UC campus faculty member, a UC graduate student, and one or two LLNL collaborators. With the recent advent of the National Science Foundation's Supercomputer Centers, even more UC faculty members have expressed interest in collaborating with LLNL staff experienced in the use of these large

Introduction

computers; about 50 UC faculty, staff, and students have been actively involved in IGPP grants in which Cray-class computing played a major role.

The Astrophysics and High-Pressure Physics Centers are located in Trailer 2177 at LLNL, near the Physics, Computations, and Defense Systems departments. The Center for Geosciences resides near the Earth Sciences complex, in Trailers 1477 and 1478. Available experimental facilities include the two-stage gas gun and diamond anvil cells, broadband digital seismic equipment, including arrays, and a variety of computational resources.

Figure 1. Distribution of mini-grant participants in the IGPP-LLNL, from FY 1983-1986.

Figure 2. Participants were balanced between UC faculty, staff, students, and also members of LLNL staff and other universities.

Figure 3. IGPP-LLNL computer users were distributed among several UC campuses.

Highlights of the 1986 Fiscal Year at the IGPP-LLNL

(July 1, 1985 – June 30, 1986)

New Center Heads for Astrophysics and Geosciences

Two new center heads came to the IGPP-LLNL in 1986. Charles Alcock, formerly at the Massachusetts Institute of Technology, will head the IGPP's Astrophysics Research Center. George Zandt, from the State University of New York, will head the IGPP's Center for Geosciences, replacing James Scheimer (who is on leave in Washington DC). William Nellis will continue to head the IGPP's High-Pressure Physics Center.

The Broadened Role of IGPP's Seismic Research Center

Over the past few years, the IGPP has seen increased interest and participation from the nuclear chemistry and geochemistry groups at LLNL. This year, when the UC Regents and the LLNL Director increased the funds available for mini-grants, it was decided to include these two areas in the IGPP's overall program. Consequently, the mission of the Seismic Research Center has been redefined to include the disciplines of geochemistry and cosmochemistry; the Seismic Research Center has been renamed the Center for Geosciences.

Four IGPP-Sponsored Workshops and Conferences

In Fiscal Year 1986, the IGPP sponsored or co-sponsored four workshops and conferences. Such sponsorship is an important way to reach out to the University community, and to make ties with potential future collaborators in our programs.

From the IGPP's perspective, the most significant of these conferences was the annual "All-University of California Astronomers' Meeting," co-hosted with the UC Davis Physics Department, which was held at LLNL in mid-May, 1986. The All-UC Astronomers' Meeting is held at a different UC campus each year; this was the first time it had been held at a National Laboratory. The meeting took place at the LLNL main auditorium, and was followed by a tour of the Nova laser facility. About 125 astronomers attended.

The IGPP co-sponsored, with LLNL's Nuclear Waste Isolation Program, the LLNL "Workshop on Geochemical Modelling" at Fallen Leaf Lake, CA, in September 1986. The IGPP also co-sponsored the workshop, "Nearly Normal Galaxies: from the Planck Time to the Present," which was held at UC Santa Cruz in July. Finally, the IGPP helped to sponsor the "Moriond Workshop on Neutrino Mass Experiments," held in January 1986.

Computer Simulation of Astrophysical Plasmas

During the past year, the IGPP-LLNL has been able to establish a particularly strong presence in the computer simulation of astrophysical plasmas and self-gravitating N-body systems. Under an IGPP mini-grant and an LLNL Institutional Research & Development project, investigators have adapted advanced computational methods developed in LLNL's magnetic and inertial fusion programs for simulating the acceleration of cosmic-rays at supernova remnant shocks, the formation of relativistic shock waves near pulsars or active galactic nuclei, and the reconnection of magnetic field in the Earth's magnetotail. In a second IGPP mini-grant and in collaboration with two joint IGPP-Berkeley post-doctoral researchers, a new "tree code" simulation model is being developed to study gravitational "plasmas" such as disk galaxies. The formation of galaxy clusters and super-clusters under the influence of cosmic strings from the early universe is also being simulated.

LLNL-UC Accelerator Mass Spectrometry Facility

During FY 1986, a group of UC researchers developed plans for an Accelerator Mass Spectroscopy (AMS) facility in California. This facility is currently under construction at LLNL, and will use a new Tandem Van de Graaf accelerator in collaboration with LLNL's E Division, R Program, and Nuclear Chemistry Department, as well as with Sandia National Laboratory at Livermore. The IGPP's systemwide administration and LLNL branch will coordinate the UC AMS effort.

Increased Mini-Grant Funds in FY 1986

Table 1 and Figs. 4 and 5 illustrate the rapid growth of UC campus interest and participation in the IGPP-LLNL's mini-grant program. The total number of proposals received has more than doubled since 1984, and the total dollars requested has risen by a factor of three.

In response to this added interest, the UC Regents and the LLNL Director increased the funds available for mini-grants from a total of \$200K in FY 1984 to a total of \$354K in FY 1986. This action enabled the IGPP-LLNL to fund 29 out of the 43 proposals received in FY 1986.

Figures 4 and 5 indicate that campus interest has continued to increase for the 1987 fiscal year. As a result of the increased proposal pressure, the IGPP has had to decrease the fraction of proposals it can fund in FY 1987.

Table 1. IGPP-LLNL Proposal History for Fiscal Years 1984-1987.

Fiscal Year	Number of Proposals Received	Dollars Requested (thousands)	Cray Hours Requested
1984	25	264	99
1985	29	343	100
1986	43	585	225
1987	55	771	234

Figure 4. The number of proposals the IGPP-LLNL receives has increased greatly over the past several years.

Figure 5. The dollars requested for mini-grants each year has grown much faster than the funding level of the IGPP-LLNL mini-grant program.

IGPP Mini-Grants for FY 1986

The following three sections describe the research done under IGPP mini-grants for FY 1986. Each description includes a summary of the experimental objectives and procedure, significance of the work, and progress during the Fiscal Year.

- Center for Geosciences
- Center for High-Pressure Physics
- Astrophysics Research Center

Center for Geosciences

Seismic Wave Propagation and Structure of the Basin and Range, Nevada

Principal Investigator: J. S. McClain (UC Davis)

LLNL Collaborator: H. Patton

UC Davis Student: Y. Dilek

Other Collaborators: K. Priestly (University of Nevada,
Reno); D. Chávez (UN Reno student)

In 1985 we organized a cooperative project to study the deep structure and seismic wave propagation in the Basin and Range region of central and western Nevada. The intent of this project was to collect and analyze data from an array of intermediate-period seismometers deployed along a 300-km profile extending away from the Nevada Test Site. This array successfully recorded a major nuclear test in December of 1985. The resulting data from that test are being analyzed at all three institutions involved in this mini-grant, with UC Davis interpreting the body-wave phases, LLNL studying the fundamental-mode surface waves, and the UN Reno primarily studying the higher-mode surface waves. By combining our results, we are deriving a more complete picture of seismic wave propagation and structure in the Basin and Range region.

Abstract

We are attempting to address the complementary problems of measuring seismic wave propagation and determining the structure in the Basin and Range region of central and western Nevada. Most seismic studies are confined to a particular seismic phase—i.e., body waves, fundamental-mode waves, or higher-mode surface waves—but we recorded all three phases in our study. Each seismic phase has its own propagation characteristics, and each is sensitive to a different part of the Earth's structure. By concurrently examining all three phases, we are deriving a more complete picture of seismic wave propagation and structure in this tectonically active region.

Objectives

Progress

Our project required the successful recording of seismic waves generated by a known source on seismometers capable of detecting a broad band of seismic frequencies over great ranges. For these known sources, we made use of underground nuclear tests from the Nevada Test Site in southern Nevada, which have the advantage that they are predictable in location and time. For receivers, we used intermediate-period seismometers with digital recorders. The 11 seismic stations were deployed along a 300-km profile, beginning 100 km northwest of the test site and extending to 400 km from the site. Whenever possible, we placed the stations within mine tunnels to reduce noise. Seismometers were placed on concrete pads to provide stability. Our 11 stations were supplemented by permanent and portable stations from the University of Nevada at Reno.

The array of seismometers was deployed from late November 1985 to January 10, 1986. While we had considerable difficulty with the array in the later stage of the deployment, the Kinibito test on December 5, 1986 was successfully recorded by most of the stations (see Figure). The recordings of this test were of very high quality, with clear arrivals of body wave and higher-mode surface waves. Note the dramatic decrease in amplitude of the first-arrival P_n waves beyond Station 5, indicating a structural discontinuity between Stations 5 and 8. Fundamental-mode surface waves were also recorded.

The data were divided between the three participating groups, and analysis is proceeding with support from the IGPP-LLNL. The work at UC Davis is concentrating on the body-wave phases, modeling these phases with synthetic seismograms for laterally homogeneous phases. Such models are almost certainly inadequate, however, and in the coming months researchers will be analyzing the data for laterally heterogeneous structures. In addition, UC Davis researchers will be combining the analysis of the surface waves and body-wave phases. The work at LLNL has concentrated on the fundamental-mode surface waves. Preliminary results have successfully revealed an effective one-dimensional structure. The data have not confirmed the expected regionalization of lithospheric structure, and the absence of clear Love waves has pre-

vented the examination of lithospheric anisotropy. At UN Reno, research during the first year concentrated on examining the attenuation characteristics of higher-mode surface waves.

Continued exploitation of the data will be fruitful, particularly as this region recently has been the target for two major multi-institutional projects (Cocorp and Passcal). Our data will complement these other studies.

Chávez, D. E., and K. F. Priestly (1986), "Measurement of Frequency-Dependent L_n Attenuation in the Great Basin," *Geophys. Res. Lett.*, **13**, pp. 551-554.

Reference

Recordings of vertical-component seismograms from the Kinibito Shot, with station numbers to the right. Arrows denote the first arrivals at Station 5 (upper) and Station 8 (lower). Note the diminished P_n amplitudes on all stations beyond Station 5.

Simultaneous Hypocenter-Structure Inversions for the Santa Barbara Channel Region

Principal Investigator: W. A. Prothero, Jr. (UC Santa Barbara)

LLNL Collaborator: J. Scheimer

UC Santa Barbara Students: J. Taylor and J. Eickemeyer

Abstract

We are attempting to determine a three-dimensional P-wave velocity structure and to provide more accurate earthquake locations for the Santa Barbara Channel region. To accomplish this, we have implemented a new raytracer into a 1981 Massachusetts Institute of Technology computer program that calculates three-dimensional hypocenter-velocity structure inversions. Subsequent testing of the new version of the program has been completed, using the Santa Barbara Channel data set. The results with the improved code are promising.

Objectives

A three-dimensional hypocenter-velocity structure inversion program (written by C. Thurber at MIT, 1981) has been implemented on the Geological Sciences Vax computer at UC Santa Barbara. This program uses local earthquake and shot locations, P-wave travel times, and an initial velocity model as input data, then solves for a more accurate velocity structure and hypocenter locations using a least-squares iterative method. The work proposed for this mini-grant was to incorporate a new exact raytracer into Thurber's program and apply it to earthquake data in the Santa Barbara Channel region and the Medicine Lakes, CA, data set from the U.S. Geological Survey and LLNL. Once this new version of the program is tested and complete, it is to be implemented on one of the LLNL Cray computers.

Progress

The new exact raytracer, which uses a simplex method of optimization to improve on the raypath calculated by Thurber's original program, has been tested and incorporated into the original computer code. These results are currently being prepared for publication. For a

velocity model believed to represent the Santa Barbara Channel region, the new raytracer corrects for travel time errors as large as 0.5 s using the Thurber raytracer for raypaths longer than 30 km.

With the Santa Barbara Channel data set, tests have been completed using the Thurber program and the new raytracer. We discovered that with the new raytracer enough information is contained in the data set to resolve an acceptable three-dimensional P-wave velocity model of the Santa Barbara Channel. Program parameters—such as damping of the design matrix, appropriate values for various raytracing parameters, and an appropriate parameterization of the initial velocity model that is consistent with the data set—have been determined. We have discovered some inconsistencies in the shot data, and are currently studying them. Once these inconsistencies have been resolved, a final three-dimensional velocity model and new hypocenter locations for the Santa Barbara Channel region will be determined.

Eikemeyer, J.E., and W. Prothero (1985), "Raytracing in a Heterogeneous Medium Using the Simplex Method," *EOS*, 66, p. 980.

Reference

Earthquake Magnitude Estimation from Initial Waveform Analysis

Principal Investigator: T. V. McEvilly (UC Berkeley)

LLNL Collaborators: H. Patton and J. Scheimer

UC Berkeley Students: K. Mayeda and J.E. Scheiner

Abstract

We have studied the possibility that information about the final size of a seismic source may be contained in the developing initial P waveform. The ability to do this would have important applications in the design of an earthquake early warning system (EEWS). Furthermore, studying the workings of such a discriminant would greatly increase our understanding of the source-rupture process: for instance, if an early waveform could forecast the final seismic source size during nucleation, this suggests that the rupture process itself is unexpectedly somehow different in the initial stages for large and small earthquakes. Our preliminary observations and analysis have yielded interesting and encouraging results. Analysis of 20 broad-band recordings of 15 earthquakes recorded at regional distances in central and northern California indicates that the time rate of change of the low-frequency spectral amplitude of the initial P wave may provide an EEWS discriminant. We have calculated a series of Fourier amplitude spectra for windows beginning at the onset of the P wave and of lengths increasing in time, simulating a real-time process. We then examine the slope of the resultant spectra vs time (i.e., the derivative) as a function of magnitude. In this preliminary study, the slopes increased in an almost linear fashion with magnitude.

Objectives

Some studies have suggested that the initial seismic P waveform may contain information about the final magnitude of an earthquake. This leads to the possibility of determining the final magnitude of a seismic source during the rupture process, which could be very useful in developing an Earthquake Early Warning System (EEWS). This source-size discriminant could allow estimation of a source size in real-time by a suitable network of receiver stations and an attendant branch network of

communications. Such a discriminant might also be applied to allow clandestine testing of underground nuclear explosions; i.e., violators of a test ban treaty hoping to hide a shot signal in a large earthquake must know that an ongoing seismic event will proceed to a sufficiently large magnitude to mask the explosion's signal. Finally, since present source theory does not indicate that such a discriminant should exist, our feasibility study may provide critical information about the source-nucleation process itself. The goal of our study is to determine the existence of such a discriminant.

Our approach is to determine the horizontal asymptote of the low-frequency level of the Fourier amplitude-displacement spectrum of the initial P wave as a function of time. An improvement over the initial method of determining the spectrum involves choosing the peak spectral amplitude of the velocity spectrum and then integrating it in the frequency domain. This general method has proven to be the most accurate. Although the initial results of these calculations were only mildly encouraging (when plotted as a function of magnitude for 14 regionally recorded earthquakes), we have since determined that we can greatly improve the result by choosing smaller incremental windows of the seismogram in the time domain and truncating the operation after six seconds. The smaller incremental windows allow for an improved regression fit of the slope of the spectrum to the data, and the truncation of the procedure after six seconds minimizes the contamination of the P-wave energy by shear waves, especially for the events located close to the recording site(s). Previously, an improved relation between the slope of the spectrum and earthquake magnitude required us to edit those events believed to be contaminated by shear-wave energy; however, our refined method requires no editing of the results (see Figure). The only exceptions to the almost linear trend of the slope vs magnitude are two recordings of the August 6, 1979 "Coyote Lake earthquake." This was, however, an anomalous case in that the two recording sites were on nodes for P-wave propagation and in the opposite direction from rupture propagation.

Progress

Reference

Scheiner, J.E. and T. V. McEvilly (1986), "Magnitude Estimation from Initial Waveform Analysis," *EOS*, **67**, p. 1111.

Graph of time derivative of low-frequency P-wave spectral level vs local magnitude. Most data fall on a linear trend, indicating the possibility of predicting the final magnitude from the initial P-waveform.

Seismic Data Telemetry via Satellite Using Spread-Spectrum Technology

Principal Investigator: J. Berger (UC San Diego)

LLNL Collaborators: J. Scheimer and N. Burr

Abstract

We are studying the feasibility of real-time satellite telemetry of seismic waveform data in support of a major seismological initiative to establish a new-generation global seismographic network. Our proposed telemetry system uses "spread-spectrum technology" to reduce the physical size and power consumption of each Earth station. A complete data-acquisition system was developed, and two of the Earth stations were installed at UC San Diego in early 1986. The system is currently undergoing testing with realistic seismic data, preparing for an actual remote field experiment possibly in the near future.

Objectives

The Science Plan for a New Global Seismographic Network, Incorporated Research Institutions for Seismology (IRIS), proposed the establishment of a new-generation global seismographic network to replace the outdated World-Wide Seismographic Station Network and to augment the several independently operated digital seismographic networks extant today. One of the key features of this proposed network is the real-time telemetry of waveform data from approximately 100 stations around the world to several data centers.

In response to early discussions and meetings of the organizers and authors of the IRIS report, we proposed to undertake a study of a new and promising technology that, we believed, would offer a practical and inexpensive way to achieve the IRIS goal. The objective of this collaborative study was twofold: to demonstrate the use of particular commercially available micro-Earth stations and to develop a satellite network design using this technology for the exchange of seismic data between seismic stations and data centers.

Progress

Our experiments have introduced a new technology to the field of seismic data transmission—a technology that is likely to radically and permanently change the way networks are operated. The principal features of this system are: low acquisition cost, low operational costs (including low channel rentals), low power consumption, and small physical size.

The system uses “spread-spectrum technology,” which has recently been introduced into commercial markets. Refined over the past 30 years in military radar and radio astronomy applications, this technology has resulted in very small Earth stations with low power requirements. The technique combines the binary data signal with a signaling rate of T_s with a pseudo-random binary sequence of clock rate $T_c \gg T_s$. This has the effect of smearing the spectrum of the transmitted radiofrequency signal with a concomitant reduction in the power density. Each unit uses its own pseudo-random binary sequence that must be known by the receiver to decode the information signal and identify the originating unit. The technique minimizes interference from other satellite or terrestrial sources by using more frequency bandwidth than conventional signals transmitted at comparable data rates. Simplex (receive-only) Earth stations with antennas as small as 1.2 m in diameter have been successfully produced in quantity, are now in routine operation in the United States, and have been demonstrated overseas.

Following many delays in obtaining licenses for the IGPP-LLNL and other remote sites, two of the Earth stations were installed at UC San Diego in early 1986. For these experiments, we developed a complete data-acquisition system to test the telemetry system with realistic seismic data and with a view toward an actual remote field experiment. This unit was based on the MK III IDA Data Logger suitably modified to operate on hardware that LLNL loaned to us for this project. Additionally, software was developed to implement the functions of the data-collection system on an existing workstation networked to IGPP lab computers.

Reference

Smith, S.W. (1986), “IRIS: Progress for the Next Decade,” *EOS*, **67**, pp. 213–219.

Seismological Studies of Core-Transition Zones

Principal Investigator: L. R. Johnson (UC Berkeley)

LLNL Collaborator: F. E. Followill

UC Berkeley Student: P. Cummins

The high-quality digital data of the Regional Seismic Test Network (RSTN) provide a unique opportunity for studying fine details of the Earth's structure using teleseismic body waves. We have collected a data set containing waves that have sampled the Earth's inner-core transition zone. This data set has sufficient bandwidth and slowness range that resolution of both elastic and inelastic properties of the transition zone are feasible. Progress has also been made on the development of wave-propagation codes that can be used to interpret the data. Our preliminary results indicate that the currently accepted models of the inner-core transition zone will have to be modified in order to explain the data.

Abstract

The high quality and broad bandwidth of data generated by the Regional Seismic Test Network (RSTN) make possible several new lines of research. The objective of the present effort is to use these data to study the transition zones between the Earth's outer and inner cores. A proper study of this transition zone requires that both elastic and inelastic effects be investigated, and the RSTN data are well suited to such studies.

Objectives

Previous studies of the transition zone suggest that it involves changes in material properties that extend over a considerable depth range, indicating that inner-core solidification is not a simple process. The goal of our research is to assemble an RSTN data set that contains waves from earthquakes that have sampled the Earth's inner-core boundary region. A second goal is to develop wave-propagation codes that are sufficiently accurate to model subtle features of the waveforms and thus resolve fine details of the transition zone. Such models should provide constraints on rheological properties of the Earth's inner and outer cores.

Progress

We have made considerable progress on both major components of the research, collecting a suitable data set and developing computer codes for calculating synthetic seismograms. We searched through the National Earthquake Information Center Event Tape archive at the Center for Computational Seismology at the Lawrence Berkeley Laboratory, looking for all deep events in the distance range $105\text{--}160^\circ$ that had good signal quality and relatively simple source time functions. Twelve events satisfying these criteria were selected (mainly in the Banda and Java Sea regions), all occurring between 1980 and the present, for which the RSTN recorded a suite of inner-core reflections ranging from pre- to post-critical. One example of such a suite is shown in the Figure. Almost all of these events were listed in the International Seismological Center catalogs as having moment tensors that favor propagation vertically downward from the source. Fortunately, eight of these events were recorded by one RSTN station located in Northwest Territory, Canada, at precritical distances, where the pulse should undergo relatively little distortion and does not itself interfere with the multiple inner-core refractions. We are presently using this phase as an empirical source time series for the Green's function evaluated at greater distances. While this procedure should have the advantage of stripping out the distortion due to the Earth's mantle, we are still investigating distortion of the precritical reflection by velocity gradients at the top of the inner core.

During the past year, extensive work has been done to develop a code for generating synthetic seismograms using the 'full-wave' technique. Within the constraints imposed by the requirement of an analytic velocity profile in the inner core, this method is capable of modeling all frequency-dependent phenomena encountered by body waves interacting with the inner-core boundary, and we are now capable of accurately calculating the body-wave pulse shapes associated with critical and grazing incidence on the inner-core boundary (e.g., the PREM model) as well as diffraction by the B caustic (see part *a* of the Figure) for frequencies up to 5 Hz.

Using the full-wave theory for seismogram modeling does however require that velocity models consist of a few layers with velocity given by an analytic function of

radius. Moreover, it does not account for the coupling between P- and S-waves that occurs in regions of high velocity gradient. Since a region of anomalously high velocity gradients is exactly the type of structure we would like to use as a model for the top of the inner core, we felt that a more complete method for seismogram computation was needed.

The reflectivity method is one way of generating complete seismograms, but its use for high-frequency core phases involves an Earth-flattening approximation with a very large number of layers, and the run time for such an algorithm would be prohibitively long even on LLNL's Cray computers. We therefore developed a hybrid method that would use the full-wave theory in the mantle and outer core, but would use the reflectivity algorithm in a 500–1000 km thick zone encompassing the inner-core boundary, where the more complete calculations were needed. Even this hybrid method required an estimated run time of 30 hours on the Cray-1; considerable work was done to vectorize and streamline the code, and we now estimate that the run time will be about three hours. Accuracy checks against both the exact solution for a homogeneous Earth and the full wave solution for the PREM model indicate that our new algorithm is accurate to within a few percent.

Cummins, P. (1986), "Core Phases Recorded by the RSTN" in *Proceedings of the 1986 RSTN/NORESS Research Symposium*, Las Vegas, LLNL Conference 8604196, p. 468-478.

References

Cummins, P., and L. R. Johnson (1986), "Synthetic Modeling of Short Period PKP Phases for Inner Core Structure," *EOS*, **67**, p. 1100.

(a) Theoretical travel time (seconds) vs distance (degrees) curves for core (PKP) and inner-core (PKiKP) phases for a standard Earth velocity model.
 (b) Seismograms of an earthquake recorded at the Regional Seismic Test Network (RSTN) are plotted at their appropriate distances and compared to the theoretical travel times (gray curve) to aid in the identification of the core phases.

Q Structure Beneath the Mono Craters-Long Valley Region of Eastern California

Principal Investigator: W.A. Prothero, Jr. (UC Santa Barbara)

LLNL Collaborator: J. Scheimer

UC Santa Barbara Student: L. K. Steck

Analysis of earthquake coda waves may yield information about the underlying geology beneath a local receiver site and about the seismic attenuation along the raypath. We have applied the single-scattering random heterogeneity theory of coda formation to local earthquakes recorded on an LLNL seismic network at Mono Craters, California. Regional values of the attenuation Q determined from these data support observations by other researchers that the frequency dependence of attenuation is proportional to the degree of tectonic activity of a region. In an analysis of site variations in coda Q , station-to-station differences were found to correlate well with underlying geology; this suggests that coda analysis may also prove to be an effective tool for aiding in the interpretation of geology beneath seismic stations.

Abstract

The coda waves of local earthquakes have been shown to be independent of source type and azimuth. This suggests that analysis of the coda may yield information about the geology beneath a local receiver site and about the seismic attenuation along the raypath. One objective of this research was to determine regional attenuation for the Mono Craters-Long Valley area in eastern California, and to compare our result with data from other regions that have been studied by the same techniques. We also attempted to determine attenuation as a function of receiver site and to investigate correlations with the underlying geology. If strong correlations exist, then coda analysis techniques offer a simple method of determining site response.

Objectives

Progress

We determined the apparent attenuation of earthquake coda waves for the Mono Craters-Long Valley region of California. Data used in this study were recorded on a LLNL digital seismic network deployed in and around the Mono Craters ring fracture zone. We analyzed the coda signals on 173 seismograms from five earthquakes located south of Long Valley Caldera, using an automated moving-window computer code. The amplitude decay was calculated by fitting the first 15 seconds of the coda to a linearized version of Sato's 1977 formula using a L-1 norm line fit.

Errors inherent in the processing code and the data were evaluated. Results from the analysis of synthetic decays show that maximum resolution of the spectral processing code is 10% of a given Q value. Data error estimations show that the quantization error is negligible, and that errors caused by ambient ground noise can usually be disregarded. The greatest source of error is noise caused by coherent late arrivals and inadequacies in the theory.

Measurements of regional apparent quality factor (Q_c) ranged from 57–473 over the frequency range of 1.5–12 Hz, with standard errors of about 35%. Receiver sites overlying crystalline rocks were observed to have higher Q_c values than those above less competent rocks. In addition, sites on or near the craters had a higher Q_c than those on Bishop Tuff to the east and south. Site differences indicate that other factors contribute to coda quality in addition to the intrinsic Q (Q_i) and the scattering Q (Q_s). A possible mechanism for site differences is the localized trapping of energy about the receiver site. Network averages for individual earthquakes indicate that attenuation is greatest for the deepest events. We interpret this result to indicate that energy from shallow events becomes trapped in the surface layers, thereby decreasing the apparent decay rate.

Efforts to separate Q_i and Q_s from Q_c show that some biasing is present in the data, possibly from multiple scattering and site effects. Because of possible data bias, Q_c results should be considered as upper bounds for this data set. Although Q_i cannot be adequately resolved, turbidity can be measured with about the same accuracy as Q_c . Turbidity for this region was found to be 0.05 ± 0.025 .

References

Sato, H. (1977), "Energy Propagation Including Scattering Effects: Single Isotropic Scattering Approximation," *J. Phys. Earth*, **25**, pp. 27-41.

Steck, L., J. Scheimer, and W. Prothero (1985), "Q Structure Beneath Mono Craters, CA," *EOS*, **66**, p. 960.

Seismic Discrimination at Small Magnitudes Using RSTN Data

Principal Investigator: T. V. McEvilly (UC Berkeley)

LLNL Collaborators: A. Smith and S. Taylor

UC Berkeley Student: R. Grose

Abstract

At present, we are unable to discriminate accurately between chemical explosions, nuclear explosions, and small-magnitude earthquakes because we do not have a clear enough understanding of their source properties and their influence on the seismic spectrum of the signals. Using seismic data of ripple-fired mining blasts acquired during the LLNL field deployment near Red Lake, Ontario, and modeling the effect of ripple-firing on the frequency spectrum, we have shown azimuthal dependence for P waves from ripple-firing. The models suggest that the spatial layout of the shot is important for frequencies greater than about 10 Hz, while the effect of random timing errors along a shot row or between rows is insignificant for frequencies greater than 50–100 Hz. The typical firing pattern will accelerate the high-frequency roll-off, while reinforcing specific high frequencies associated with the row delays.

Objectives

At present, it is difficult to detect possible test-ban treaty violations at low yields because we are unable to discriminate between the seismic signals of small-magnitude earthquakes and chemical or small nuclear explosions. One avenue of research is to study the effect on seismic spectra of “ripple-fired” mine shots—i.e., when separate rows of explosives are detonated within short time intervals (9–17 ms in this case). We have modeled the effect of ripple-fired mine shots on the signal spectra, and then compared the modeled spectra with actual high-frequency seismic data taken from the LLNL field deployment at Red Lake, Ontario. The Figure shows an example of the P_n spectrum, taken at 380 km from a mine shot in northern Minnesota. The rapid roll-off of the spectrum above 10 Hz (proportional to ω^{-4} in displacement amplitude) may result from attenuation along the propaga-

tion path; this might also be influenced by the ripple firing, as one objective of ripple firing is to minimize damage to adjacent structures by suppressing frequencies lower than 20 Hz. A second mine blast showed a feature that is often characteristic of ripple firing—strong reinforcement at specific frequencies (e.g., 30 Hz).

Progress

To account for these features and to ascertain the possibility of evading detection for test-ban treaty violations (by trying to disguise small-yield nuclear tests as ripple-fired mine shots), we have developed a procedure to model ripple-fired mine shots. The actual configuration of a particular mine blast is used to sum the effects of individual shots with delays ranging from 9–17 ms. The resulting interference of the wavefronts from individual shots depends upon both the azimuth and frequency. Here, we have calculated only the deviation of the ripple firing at two different azimuths (251 and 341°) on the power spectrum of an individual shot of 2000 pounds; the actual power spectrum would be the product of the deviation spectrum and the power spectrum of an individual shot. The effect of ripple-firing is to increase the roll-off between 10 and 20 Hz by ω^{-2} in displacement amplitude, and to reinforce frequencies associated with the principal delay time (e.g., 17 ms or approximately 60 Hz). If the original explosion rolls off as ω^{-2} at high frequencies, the ripple-fired shot would then decay as ω^{-4} , as observed. We do not observe reinforcement near 60 Hz, presumably due either to interference from 60-Hz power lines or seismic attenuation. The reinforcement at 30 Hz observed in the second blast originated from a longer (35 ms) delay between the rows; however, we have not determined, as yet, the precise firing pattern of the mine blast. Further details and confirmation of our results will be possible after we have modeled additional mine blasts.

P_n spectrum from a mine shot in northern Minnesota.

Study of Complex Rupture Patterns Along the Calaveras Fault Using Broadband Digital Seismogram Data

Principal Investigator: K. C. McNally (UC Santa Cruz)

LLNL Collaborator: J. Scheimer

UC Santa Cruz Students: G. Nelson and E. Brown

We determined seismic attenuation in the Livermore Valley by studying coda Q to determine if significant site and path variations exist. Some researchers have suggested that such variations may occur in source areas as a precursor to moderate and large earthquakes. To investigate this, we analyzed microearthquakes recorded by the Lawrence Livermore East Bay Seismic Network; our analysis used a moving-window spectral analysis program that employed a quantitative RMS amplitude determination and error estimation. We found that values of coda attenuation Q for our study area are consistent with values found for the Stone Canyon (CA) area, but are below regional values of the eastern U.S. Comparisons between groups of stations with similar local receiver geology did show a qualitative correlation between geology and attenuation, but the differences in Q values are not statistically significant.

Abstract

The Lawrence Livermore East Bay Seismic Network covers the Livermore Valley with 34 stations spaced at intervals of 5–15 km in an area roughly 80 km N-S and 50 km E-W. Two distinct geological terrains are enclosed in our study area: Franciscan and Great Valley.

Objectives

We are studying coda attenuation Q as a function of frequency, $Q_c(f)$, in the Livermore Valley to determine if significant site and path variations exist. Our results will form the basis from which temporal variations in coda Q can be investigated. Jin and Aki (1986) have suggested that such variations occur in source areas prior to moderate and large earthquakes. Our initial results show a frequency-dependent coda Q that is consistent with values found for Stone Canyon, CA, but below regional values for the eastern U.S. (see Figure). Comparison between groups

of stations with similar surface geology showed a qualitative correlation between geology and attenuation; however, the difference in Q values does not appear to be statistically significant.

Progress

The coda Q computer program and affiliated software now works with SAC (Seismic Analysis Code) both on the Livermore Prime P3 computer and at UC Santa Cruz on the Vax/VMS. Coda Q is determined for all stations picked by either the NEWT automatic picker or by the investigators. Our current procedure is to retrieve desired events from LLNL daily tapes, plot traces, and then do noise and signal spectral analysis for unusual traces. We determine $Q_c(f)$ in five frequency bands for all usable traces, eliminate $Q_c(f)$ values in noisy bands, and finally perform further analyses using the statistical language "S" on UNIX.

A plot of the inverse attenuation against the seismic wave frequency shows differences in regions from the Livermore Valley [triangles] to Stone Canyon (CA) [squares], and New England [circles].

Determination of Crustal Structure at Long Valley from Teleseismic Converted Energy

Principal Investigator: W. A. Prothero, Jr. (UC Santa Barbara)

LLNL Collaborator: G. Zandt

UC Santa Barbara Student: L. K. Steck

Abstract

The periodic eruptions in the Inyo Domes, and the intense seismicity and ground uplift in the Mammoth Lakes area over the last few years, have led some researchers to suggest that magma may exist approximately 6 km beneath the Long Valley caldera. The available data are very limited and somewhat inconclusive, largely because of the types of seismic sources that have been used, such as explosions and local earthquakes. We are testing a new teleseismic technique that uses three portable digital broadband seismic instruments to measure the conversion of P and S wave seismic energy in an area. By deploying a seismic network around the resurgent dome in the caldera, it is possible to map the magma bodies in three dimensions. Our method requires only one recording station to determine crustal structure directly beneath a given site. Because of the great sensitivity of this approach to contrast in shear velocity, it offers a promising technique for resolving low-shear-velocity bodies such as magma. To date, we have occupied four sites and have recorded sufficient data for our analysis. We will make an assessment of the broader applications for this teleseismic technique to study deeper upper-mantle structures.

Objectives

Seismic studies in the Mammoth Lakes area of California suggest that one or more magma bodies may exist at depths of approximately 6 km beneath the resurgent dome in Long Valley Caldera. The evidence in these studies for the location and configuration of the magma bodies is very limited and somewhat inconclusive, since the only types of seismic sources used have been explosions and local earthquakes. However, the use of portable broadband triggered instruments to study P-S converted teleseismic waves offers a simple and direct method of determining the three-dimensional extent of crustal features.

We intend to test this technique for mapping, in three dimensions, the magma bodies thought to exist beneath Long Valley Caldera, and to examine the method's applicability to the study of deeper upper-mantle structures.

Progress

We have deployed three portable digital broadband seismic instruments around the resurgent dome in Long Valley Caldera. These three-component, triggered instruments have a flat response between 0.1 and 10 Hz and produce very high-quality data. Four sites have been occupied over the course of about six weeks. We chose two sites, located in Sand Canyon and at an abandoned drill pad, because of evidence in support of magma at depth beneath them. The third site, with no evidence of magma beneath it, was chosen as a control site. This control site proved to be extremely noisy, possibly because of thick layers of lake sediments, and we therefore moved to a much quieter site closer to the resurgent dome.

Although the instruments had been previously deployed in the Mojave desert for three months, new triggering parameters were required for the Long Valley array. We attribute this to the occurrence of numerous aftershocks from the Chalfont Valley earthquake (15 km east of Long Valley), and to the presence of thick lake bed deposits in the caldera, both of which caused an increase in noise levels at Long Valley.

The following table summarizes the data recorded to date for each site.

Site No.	Instrument	No. of Teleseisms	M Range
1	Ampere	17	5.0–6.5
2	Cavendish	20	4.8–6.5
3	Boyle	6	4.8–6.5
4	Boyle	8	4.9–6.3

Each channel of each instrument must be well calibrated. To accomplish this, we have been adapting an *in-situ* random binary telegraph calibration technique from Sauter and Dorman. After completing this, we will group the data according to azimuth and distance, and we will polarization filter it to enhance P-S energy. Time delays between the direct P and the converted S energy will be used to model crustal and upper-mantle velocity structures. We will also use an inversion technique developed by Owens et al. (1984) to determine crustal structure.

Owens, T., G. Zandt, and S. Taylor (1984), "Seismic Evidence for an Ancient Rift Beneath the Cumberland Plateau, Tennessee: a Detailed Analysis of Broadband Teleseismic Waveforms," *J. Geophys. Res.*, **89**, pp. 7783-7795.

References

Sauter, A. and L. M. Dorman (1984), "Ocean Bottom Seismometer Calibration on the Sea Floor: Instrument Effects," unpublished manuscript.

Prothero, W. (1986), "A Portable, Broadband Triggered Teleseismic Recorder," *EOS*, **67**, p. 316.

Dynamic Response of Fully and Partially Fluid-Saturated Rocks

Principal Investigators: W. Goldsmith and M. M. Carroll
(UC Berkeley)

LLNL Collaborators: B.P. Bonner and R.C.Y. Chin

UC Berkeley Students: A. Imam and B. Revisn

Abstract

Previous research in studying the dynamic response of rocks has been generally devoted to the investigation of dry rocks; in the field, however, many strata are either partially filled or saturated with various types of fluids. Our principal interest is to determine the effect of fluid saturation on the constitutive equations, on the microscopic deformation behavior, and on the wave-propagation process. To properly interpret our experimental results, we are generalizing the theoretical pore-collapse model for dry porous materials to include fluid-filled pores. This will allow proper phenomenological and analytical modeling of the response of various types of rocks to transient loads, and will permit predictions of the history of mechanical field variables at distant positions from the loading zone; also, we will be able to study the propagation of waves in a pre-stressed fluid-saturated porous medium. Our results will be useful in evaluating the vulnerability of both surface and underground structures subjected to the seismic loading, in the detection of underground explosions, and in the exploration of new energy resources.

Objectives

We used two gas guns at UC Berkeley for Hopkinson bar and split Hopkinson bar experiments to obtain stress-vs-strain data at strain rates up to $10^3/s$. To obtain dry specimens, rocks were heated in a vacuum chamber. We immersed the fluid-filled rock specimens in fluid to saturate the pores; these specimens were also immersed during the dynamic experiments. We recorded the outputs of strain gauges and piezoelectric stress transducers on digital oscilloscopes with a time resolution down to 20 ns. At LLNL, we performed digital image processing of scanning electron microscope (SEM) and acoustic micrographs, as well as characterization of porosity, internal surface area, and ultrasonic wave propagation, on the

same set of specimen materials. The equations for pore collapse with fluid inclusions will be solved with initial and boundary conditions corresponding to the Hopkinson bar experiments. Our effort is concentrated in the linear response regime to study intrinsic material dissipation and dispersive mechanisms that interact with the geometric dispersion effect.

Split Hopkinson bar experiments have been performed on 17 specimens of dry Nugget sandstone at stresses between 22,000–29,000 psi. The static properties of this rock, known from previous tests at LLNL, are needed to apply critical-state plasticity theory. From these data, we are deriving the constitutive relations for this rock under dynamic uniaxial deformation. Further work will be performed using the same rock with fluid-filled pores.

Progress

Ion Chromatographic Analysis of Ice Core Samples from Central Greenland

Principal Investigator: H. Craig (UC San Diego)
LLNL Collaborator: R. Finkel

Abstract

We are preparing to use the accelerator mass spectrometry (AMS) facility currently under construction at LLNL to study the history of cosmogenic isotope production as recorded in the ^{10}Be and ^{36}Cl content of polar and high-altitude ice sheets. The information gathered from this work will help us to understand the history of the cosmic ray flux, the periodicity of the 11-year solar sunspot cycle, variations in the geomagnetic field, and variations in global atmospheric circulation. In order for us to interpret the isotopic measurements, we must coordinate our AMS measurements with measurements of the chemical composition of the ice cores. Preliminary chemical composition measurements have been carried out.

Objectives

Polar and high-altitude ice sheets, such as those found in central Greenland, contain pristine records of Earth's historical climatic conditions. Three factors may influence the concentrations of cosmogenic isotopes in precipitation, as found in polar ice samples: variations in the primary cosmic ray flux, variations in the solar or terrestrial magnetic field (which would affect the incoming cosmic ray particles), and variations in atmospheric circulation (which would redistribute cosmic-ray products). We are preparing to use the accelerator mass spectrometry (AMS) facility currently under construction at LLNL to study the history of cosmogenic isotope production as recorded in the ^{10}Be and ^{36}Cl content of polar and high-altitude ice sheets. Our investigations should provide insight into basic physics problems, such as the history of the cosmic-ray flux, the 11-year periodicity of the solar sunspot cycle, variations in the Earth's magnetic field, and variations in global atmospheric circulation.

In order to separate meteorological effects from production-rate effects, it will be necessary to combine the

AMS measurements of isotopic concentrations with ion chromatographic determination of the chemical composition of the ice cores.

Progress

As groundwork for this effort, the ion chromatograph at the Scripps Institution of Oceanography at UC San Diego was reconfigured to attain the high sensitivity required for ice core analyses. We analyzed several samples of Antarctic ice from the Allan Hills region—which had been collected in conjunction with Antarctic meteorites—for chloride, nitrate, and sulfate concentrations. These analyses confirmed our ability to attain the requisite sensitivity (1 ppb), and also provided data for interpreting the ^{36}Cl measurements made on these same samples.

Originally, we had planned to study geographical variations in precipitation chemistry over Greenland by comparing new analyses of cores from central Greenland with previously measured results from southern Greenland. However, ice core material for this study has not yet been available. Nevertheless, we have laid a good foundation for continued work. When the LLNL AMS facility comes on line, probably within the next 12 months, we will be ready to implement an ice-core analysis program; in the interim, we have undertaken two studies:

- We have received 12 ice samples from the Dundee ice sheet in China for ^{10}Be and ^{36}Cl analysis. This mid-latitude, high-altitude ice sheet samples a different atmospheric regime than those represented by the Greenland and Antarctic ice sheets, and will provide information about the role of atmospheric circulation in redistributing atmospheric spallation products.
- We will shortly begin chemical analysis of Antarctic ice samples from the Allan Hills region; these samples, currently in cold-storage at the Scripps Institution of Oceanography, are from a sublimation region of the ice sheet and will give information both on the composition of old ice and on possible post-depositional alteration of the chemical composition of the ice pack.

Study of Heat Flow in the Salton Sea Geothermal Area and Its Adjacent Fault Zones

Principal Investigator: T. C. Lee (UC Riverside)

LLNL Collaborator: P. W. Kasameyer

UC Riverside Student: Z. Yi

Abstract

We have analyzed temperature logs and measured the thermal conductivity of drill cuttings to determine the heat flow in the offshore area of the Salton Sea geothermal field. We found that most of the sites are dominated by conductive heat transfer, but at a few sites, temperature profiles reveal the strong influence of fluid flow. Conductivity distribution is bimodal, with the higher mode corresponding to silty sand and the lower mode corresponding to silty clay. The area offshore is characterized by high heat flow ($> 0.1 \text{ W/m}^2$). Two areas with extremely high heat flow ($> 1.5 \text{ W/m}^2$) are found near Mullet Island and about two miles southwest of the Obsidian Butte. We found that the overall Salton Sea thermal anomaly is not symmetric with respect to the arc of volcanic domes, as had been previously thought without the temperature data.

Objectives

The Salton Sea geothermal field (SSGF) contains the largest known geothermal resource in Southern California's Imperial Valley. Previously, assessment of the offshore portion of the SSGF has been limited to gravity and aerometric data, because no drill holes had been made under the lake water. We are evaluating the coherence of temperature data collected from offshore drill holes, and are also measuring the thermal conductivity of drill cuttings; this will help us to delineate the thermal anomaly from offshore and on-land heat-flow data. Ultimately, this study should provide thermal data for accurate resource assessment and for thermal modeling of the geothermal field; we may also be able to relate the thermal anomaly with tectonic activity in the area.

We studied two sets of temperature logs (from the Bear Creek Mining Company and from a study by LLNL and Sandia National Laboratories) to examine heat flow in the offshore portion of the SSGF. Temperature logging has been made several times at individual sites, but the data collected by the Bear Creek Mining Company appear to be less coherent than the set measured by LLNL and Sandia. Upon studying the temperature data, we find that most sites are dominated by conductive heat transfer. At a few sites, the temperature profiles are disturbed by loss of drill mud (to permeable layers) or groundwater movement. Using the characteristics of temperature profiles and temperature recovery rates, we are attempting to quantify the influence of fluid flow on the temperature profiles.

At each site, we then measured the thermal conductivity of drill cuttings and core samples at about 3-m intervals with a technique newly developed at UC Riverside. Shorter sampling intervals were taken when we found a large change in conductivity. The Figure depicts the bimodal distribution of conductivities for all samples. The higher-mode ($1.9 \text{ W/m}^2\text{K}$) corresponds to silty sands, while the lower mode (about $1.0 \text{ W/m}^2\text{K}$) corresponds to silty clay.

Preliminary results indicate that the areas off the volcanic domes are dominated by high heat flow ($> 0.1 \text{ W/m}^2$). We have identified two areas with extremely high heat flows ($> 1.5 \text{ W/m}^2$), one near Mullet Island and the other about two miles southwest of the Obsidian Butte. We are not certain if a relation exists between these two anomalies and the San Andreas fault and Brawley fault (other than geographic proximity). Overall, this study suggests that the offshore thermal anomaly is not as extensive in area as the on-land portion, nor is it symmetric with respect to the volcanic domes, as had been envisioned earlier.

References

Lee, T-C., T. L. Henyey, and B. N. Damiata (1986), "A Single Method for the Absolute Measurement of Thermal Conductivity of Drill Cuttings," *Geophysics*, **51**, pp. 1580-1584.

Newmark, R. L., P. W. Kasameyer, L. W. Younker, and P. C. Lysne (1986), "Research Drilling at the Salton Sea Geothermal Field, California: The Shallow Thermal Gradient Project," *EOS*, **67**, pp. 698-707.

Histogram of thermal conductivities of drill cuttings. Note the two distinct modes, corresponding to silty clay (left) and silty sand (right).

Center for High-Pressure Physics

Emission Spectra from Simple Shocked Solids

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

LLNL Collaborator: N. C. Holmes

UC Los Angeles Collaborator: M. L. Johnson (now staff research associate at Division of Geological and Planetary Sciences, California Institute of Technology) and S. Johnson

We are using the LLNL two-stage light-gas gun to study chemistry during shock compression of simple organic molecules (CO , CH_4 , N_2 , C_6H_6 , $\text{C}_6\text{H}_5\text{N}$) and of a "planet-in-a-bottle" solution of isopropanol, ammonia, and water with C:N:O compositions of cosmic abundance. Our experiments were conducted at pressures relevant to interiors of the giant planets where shock equations of state, conductivity studies, and static data indicate that such molecules undergo chemical reactions. We have shown by emission spectra from the shock front that excited C_2 molecules are formed during single- and double-shock decomposition of benzene at pressures from less than 20 GPa (200 kbar) to more than 70 GPa. Decomposition seems not to proceed directly to equilibrium compositions of hydrogen and graphite or diamond, as has been suggested by some models. Our double-shock experiments also indicate that the kinetics of reactions can be followed behind the second shock front.

Abstract

We are attempting to demonstrate the value of molecular electronic or vibrational emission spectroscopy for analyzing the chemistry of shock decomposition in simple molecular systems. Shock-wave studies of simple carbon compounds, such as CO , C_6H_6 , and N_2 , suggest that these materials decompose at high shock pressures. CO also decomposes at moderate static pressures, and more complex organic compounds are expected to decompose during shock compression. Shock Hugoniot data,

Objectives

however, do not provide information about the extent of decomposition; the interpretations of the shock data depend critically on assumptions about the products formed, their equations of state, and their rates of formation. Molecular spectra provide ways for us to detect and identify the products and intermediates of shock-decomposition reactions. In favorable cases, the kinetics of reactions behind the shock front can also be determined by spectroscopy.

Progress

During previous years, targets for the LLNL two-stage light-gas gun were designed, then coupled to intensified, gated, optical multichannel analyzers (OMAs), which detect the emission spectra. These target designs were tested successfully during early FY 1985 with a series of experiments using benzene samples. These data showed that benzene emitted much more strongly than we had anticipated, and that more detailed optical diagnostics could be added to the apparatus. We tested several of these additions during FY 1986, and more tests are planned for FY 1987. The early benzene studies also demonstrated that we did not need to synthesize compounds that are known to decompose with high yields of chemiluminescence.

Experiments with shock-compressed benzene conducted during the last two years have shown that very strong molecular emission spectra accompany shock decomposition. Bands characteristic of the Swan system of C_2 occur with various relative intensities and vibrational shadings at pressures as high as 70 GPa. Several ultraviolet features have been observed at some pressures, but these are less reproducible, and have not been identified. Sharp bands in many spectra are also detected, which appear to be associated with atomic impurities. The C_2 data indicate that the decomposition mechanisms at high pressures are qualitatively similar, but much faster, than benzene pyrolysis near atmospheric pressure. The 13-GPa feature in the equation of state represents the transition from phenyl radical chemistry to ring-opening chemistry. During 1986, we extended these experiments to include a benzene derivative, benzonitrile, which should allow us to probe additional shock-decomposition channels of the benzene ring system.

Recent experiments have included two or three OMA systems and several photomultipliers (PMTs). One OMA is gated to obtain emission spectra over broad wavelength regions from the single-shocked material, another is gated to obtain spectra from double-shocked material; the PMTs follow the temporal evolution of the emission at specific wavelengths throughout the passage of the initial and reflected (double) shock over an interval of several microseconds. OMA spectra and PMT data of the emission near 515 nm obtained during our first two successful double-shock experiments showed that the kinetics of emitting species behind the reflected shock front can be followed with multiple detectors. The Figure shows sample PMT data from a double-shock experiment. These results suggest that we may be able to use reflected-shock methods to detect absorption by species that do not emit.

Another component of this study investigates organic chemistry during shock compression of a synthetic "planet-in-a-bottle" mixture. Work has begun with an experimentally convenient solution of isopropanol, ammonia, and water with C:N:O compositions of cosmic abundance. We will also study other starting mixtures involving alkyl amines, alcohols, and water in order to determine whether the results depend strongly upon the initial chemical species. Shock equation-of-state data for this mixture at pressures relevant to interiors of the giant planets were obtained. In future experiments, we will measure the electrical conductivity of this compressed mixture and look for molecular emissions from the hot, compressed material that may help us to identify its molecular composition.

Holmes, N. C., W. J. Nellis, W. B. Graham, G. E. Walrafen, M. L. Johnson, and M. Nicol (1985), "Experimental Spectroscopy on Planetary Ices at Extreme Conditions," *EOS*, 66, p. 948.

References

Johnson, M. L., M. Nicol, and N. C. Holmes (1986), "Molecular Emission Spectra from Shock-Decomposed Benzene," *Shock Waves in Condensed Matter*, Y.M. Gupta, Ed. (Plenum, New York) pp. 201-206.

Nicol, M., M. L. Johnson, and N. C. Holmes (1986), "Chemiluminescence of Shock-Pyrolyzed Benzene," *Physica B*, **139/140**, pp. 582-586.

Nellis, W. J., D. C. Hamilton, N. C. Holmes, A. C. Mitchell, H. B. Radousky, F. H. Ree, M. Ross, and M. Nicol (1986), "Properties of Materials in the Interiors of Uranus and Neptune," presented at Lunar and Planetary Sciences Conference XVII, Houston, March 1986.

N. C. Holmes, M. Nicol, and M. L. Johnson (1986) "Emission Spectroscopy of Shocked Benzene," presented at Gordon Research Conference on Research at High Pressures, Meriden, NH, June 1986.

Some of this research was also presented at the 1986 Annual LLNL/LANL Exchange on High Explosive Technology, July 1986.

Photomultiplier data from a benzene emission spectroscopy experiment. The upper trace is the time-resolved intensity of the emission centered in a narrow band about 598 nm, a region that does not contain a Swan band and is most sensitive to greybody emission. The lower trace is from a channel centered at 506 nm, near the center of a Swan band of C. The first plateau in the data after the initial rise shows that the emission intensity in both bands is nearly constant during the time the first shock traverses the benzene sample. The sharp second rise in both traces occurs when the first shock arrives at the window, sending a reflected shock wave back into the sample. The upper trace shows that the thermal emission from the sample is constant until the first shock reaches the rear surface of the window. The lower trace shows a marked time dependence during this interval, which may indicate the effects of chemical kinetics on the formation and decay of C molecules.

Statistical Mechanics and Phase Equilibria of Ionic and Geophysical Systems at High Pressure

Principal Investigator: M. S. T. Bukowinski (UC Berkeley)

LLNL Collaborator: M. Ross

UC Berkeley Student: G. H. Wolf

Abstract

We are investigating the high-pressure / high-temperature thermoelastic properties of solid and liquid phases of ionic minerals through a combination of numerical simulations, first principles, and ab initio theoretical methods. We have used Modified Electron Gas (MEG) pair potentials in a very successful attempt to model the structural and thermal properties of MgSiO_3 perovskite, MgO , and CaO , as functions of pressure and temperature. Melting of KCl , and its relationship to lattice instability have been analyzed with a Monte Carlo code developed at LLNL. The same code, together with MEG pair potentials, has yielded extremely accurate thermal properties of MgO . However, the modeling of elastic constants requires the addition of many-body effects, and we have therefore developed a new variational electron density pair-potential model that includes ionic self energies; this model yields equations of state and elastic constants that agree much better with existing data than those obtained with MEG pair potentials.

Objectives

The properties of liquids and minerals at high pressures and high temperatures play an important role in the thermal and chemical evolution of the inner planets. These properties are not well understood, however, for silicate minerals and their melts. Recent developments suggest that at pressures corresponding to the upper mantle of the Earth, some silicate melts become denser than the solids with which they are in equilibrium, implying that melts generated deep in the mantle will sink. Work on high-pressure phase equilibria of silicate minerals has demonstrated that the perovskite phase is obtained at pressures above 25 GPa, and it is therefore important to understand the structural stability and thermodynamic properties of MgSiO_3 perovskite throughout the Earth's

lower mantle. We are developing both qualitative and quantitative theoretical methods of modeling the high pressure/high temperature properties of ionic solids and melts to illuminate the physics of these materials and to provide quantitative estimates of their equations of state, elastic constants, and structure.

Successful modeling of minerals for which little or no high-pressure data exist relies rather heavily on physical models of ionic interactions. Hence, the first part of our project deals with testing and developing reliable pair potentials. We chose the pair-potential approach because of its flexibility, which would allow us to compute a variety of thermodynamic and structural parameters. We found that the Modified Electron Gas (MEG) pair potentials give excellent compressibilities and thermal expansivities, but tend to underestimate the equilibrium densities of oxides. Furthermore, since they are central pair potentials, these numbers cannot yield accurate elastic constants other than the bulk modulus. We have developed several versions of MEG pair potentials, the most successful of which is based on a variationally stabilized oxygen ion that accounts for the dependence of the self energy of the ion on the crystal structure. Many-body effects are thus included. Calculations for MgO and CaO show that our method gives fairly accurate elastic constants.

Progress

We are also developing lattice-dynamics codes that use force constants based on the pair potentials developed earlier. We completed a major code that can compute the phonon spectrum of orthorhombic lattices with internal degrees of freedom in a thermally self-consistent way. This code was used for a detailed analysis of the structure and equations of state of several perovskite-type minerals. Our calculations predict that pressure or temperature increases or decreases the degree of distortion, respectively, of MgSiO_3 perovskite, in contradiction with earlier predictions based on simple ionic-compressibility concepts. Our predictions regarding the pressure effects have since been confirmed experimentally. The new calculations also predict that increasing temperature will cause critical phase transformations that are analogous to those observed in NaMgF_3 perovskite. If real, these transformations have significant geophysical consequences. Also of

geophysical significance are our computed equations of state, which match available low-pressure data very well.

We have also begun modeling high-pressure ionic liquid structure and anharmonic properties of solids. After carrying out a Monte Carlo simulation of liquid and solid KCl, we found that lattice instabilities predicted by quasi-harmonic lattice dynamics do not give reliable estimates of melting temperatures, as has been suggested in some recent publications. We used our Monte Carlo code to test the MEG pair potentials in the calculation of thermal expansivity, obtaining excellent results for MgO by duplicating the experimentally determined temperature dependence of the volume and compressibility. Our calculations also show that anharmonicity has a negligible effect on the thermodynamics of MgO at pressures and temperatures corresponding to the lower mantle of the Earth, which has been confirmed in shock-wave experiments. These results have allowed us to construct more reliable estimates of the mineral composition of the lower mantle.

This Monte Carlo code has been adapted to simulate constant-pressure ensembles of ionic liquids. Preliminary work has been done on liquid and glassy SiO₂, using parameetric pair potentials. The simulations are able to produce a glass transition upon cooling of the liquid. The glass-transition temperature, however, is too low by about 30%, and the thermodynamic properties are not very accurately reproduced. Further progress will rely on improved pair potentials.

References

Bukowinski, M.S.T. and G. H. Wolf (1985), "Implications of the Thermoelastic Properties of MgSiO₃ Perovskite on Lower Mantle Compositional Models," *EOS*, **66**, p. 1057.

Bukowinski M.S.T., and G.H. Wolf (1987) "Thermoelastic Properties and Possible Critical Transitions in MgSiO₃ Perovskite at Lower Mantle Conditions," *Structural and Magnetic Phase Transitions in Minerals*, S. Ghoses, J. M. D. Coey, and E. Salje, Eds. (Springer-Verlag, Berlin — in press).

Ross, M., and G. H. Wolf (1986), "High-Pressure Melting Curve of KCl: Evidence against Lattice-Instability Theories of Melting," *Phys. Rev. Lett.*, **57**, p. 214.

Wolf, G. H., and M. S. T. Bukowinski (1985), "Ab Initio Structural and Thermoelastic Properties of Orthorhombic MgSiO_3 Perovskite," *EOS*, **66**, p. 1057.

Wolf, G. H., and M. S. T. Bukowinski (1986), "Theoretical Study of the Structural and Thermoelastic Properties of MgSiO_3 and CaSiO_3 Perovskites: Implications for Lower Mantle Composition," presented at the 1986 U.S.-Japan seminar on High Pressure Research: Applications to Geophysics and Geochemistry, M. Manghnani and S. Akimoto, Eds. (in press).

Wolf, G. H., and M. S. T. Bukowinski (1987) "Variational Stabilization of the Ionic Charge Densities in the Electron-Gas Theory of Crystals: Applications to MgO and CaO ," *Phys. Chem. Minerals* (in press).

Melting of Simple Solids at High Pressures

Principal Investigator: R. Boehler, (UC Los Angeles, now at the Max Planck Institute, Mainz, West Germany)

LLNL Collaborators: M. Ross and D. A. Young

UC Los Angeles Collaborators: Z. Chang-Sheng (now at the Geophysical Laboratory of the Carnegie Institution) and M. F. Nicol

Abstract

Melting is a delicate balance between two phases of matter, solid and liquid. Since theoretical melting curves are very sensitive to errors in the statistical mechanical models of either the solid or liquid phase, accurate determinations of the melting curves of materials at high pressures provide detailed challenges of current theory. Thus, predicted melting curves are very sensitive tests of statistical mechanical models for both phases. We have shown that excellent agreement can be obtained for the theoretical and experimental melting curves of several simple atomic systems. During 1986, we extended our experiments from monatomic argon to a diatomic molecular solid, nitrogen, following its melting curve above 10 GPa.

Objectives

Accurate determinations of the melting curves of materials at high pressures provide sensitive tests of statistical mechanical theories of the solid and liquid states. Theoretical melting curves are very sensitive to errors in the statistical mechanical models of either the solid or the liquid phase. We have studied the melting of several simple materials in the diamond-anvil cell at high pressures to obtain results of sufficiently high accuracy to challenge the theoretical studies being conducted at LLNL of the relevant fluids and solids.

Progress

Detailed theoretical predictions were available for the class of inert gas elements. An understanding of the melting properties of these elements and other simple molecular solids is important for understanding the structures of the major planets. We developed a simple interferometric method to detect the melting of these solids in externally heated diamond-anvil cells. We demonstrated

the accuracy of our method by extending the melting curve of argon to 60 kbar and about 750 K; this more than doubled the reported melting range of argon. Our measurements are in excellent agreement with the theory concurrently developed at LLNL.

Below 35 kbar, we detected melting by observing the disappearance of the crystal grain boundaries. The melting temperatures and pressures were taken when the crystals were in equilibrium with the fluid. At higher pressures, grain boundaries were difficult to detect, and we measured melting by monitoring an interference pattern for light transmitted through the diamonds and sample. The first Figure shows an optical signal recorded during a temperature scan through the melting transition. The sharp discontinuity results from the differences between the refractive indices of the solid and liquid. This work is limited to temperatures below 750 K because the ruby luminescence technique for pressure determination fails at higher temperatures.

Success with atomic solids motivated us to extend these studies to the next most complicated case, diatomic molecular solids. We decided to work with nitrogen because it is easier to treat theoretically than other diatomics. The nonsphericity of the nitrogen molecule adds another element of complexity to the theory already developed for argon. When this work started, the only nitrogen melting data had been measured in piston-cylinder apparatus up to 2.8 GPa.

We also used the interferometric and direct visual techniques developed for argon to extend the nitrogen melting curve to the delta-beta-liquid triple point at 580 K and 9.9 GPa, which (within experimental error) is at the point reported in the literature. Above the triple point, it was difficult to detect melting by either interferometry or direct observation; however, we could detect melting for about another 100 K by observing the light scattered by the fluid-solid mixture.

We developed satisfactory theoretical fits of the nitrogen melting curve by extending a spherically-averaged potential model, similar to that used for atomic solids, to take the diatomic's free energy of rotation or

libration explicitly into account. An example of this is shown in the second Figure. The librational contribution in the solid was parameterized in terms of an effective rotational Debye temperature and Gruneisen parameter. The fitted values of the parameters can be explained in terms of realistic estimates of the energy barriers that perturb rotation in the solid phase.

References

Zha, C. S, R. Boehler, D. A. Young, and M. Ross, (1986), "The Argon Melting Curve to Very High Pressures," *J. Chem. Phys.*, **85**, p. 1034.

Young, D. A., C. S. Zha, R. Boehler, A. S. Zinn, J. Yen, M. Nichol, D. Schiferl, S. Kincaid, R. C. Hanson, and D. Pinnick (1987), "Diatomic Melting Curves to Very High Pressure," *Phys. Rev. B.*, **35**, pp. 5353-5356.

Interferogram from a determination of the melting point of argon in a diamond-anvil cell at high pressure and temperature. The abrupt intensity change occurs at the melting point.

The melting temperature of N_2 as a function of pressure. The triangles are our experimental data. The solid curve is our theory (1 GPa = 10 kbar).

Deformation-Enhanced Dissolution in Theory, Experiment, and Nature, Based on Microstructural Evidence

Principal Investigator: H.R. Wenk (U.C. Berkeley)

LLNL Collaborator: H.C. Heard

UC Berkeley Student: A. Meike

Abstract

Rocks that have deformed under certain conditions of high pressure can exhibit evidence of a heterogeneous diffusive mechanism of mass transfer, often called "pressure dissolution." To investigate the phenomena of pressure dissolution, we are using transmission electron microscopy (TEM) to study the microstructures associated with solution cleavage in the Scaglia Rossa limestone from the Umbria-Marche Apennines, Italy. The TEM-resolved dislocations were concentrated within limited areas of single grains. Comparisons with experimentally deformed calcite microstructures and with computer simulations of TEM dislocation contrast allowed the interpretation of the character and density of these dislocations. Our results suggested that selective dissolution of localized dislocation tangles was responsible for solution cleavage formation. Solution cleavage may be unique to the transition zone between fracture and flow styles of deformation, where grains have the greatest potential for heterogeneous deformations. This summary focuses on the limestone microstructures, but also describes some phyllosilicate features.

Objectives

Our calcite strain-dissolution experiments are one part of an attempt to reproduce microstructures observed in association with solution cleavage in limestone under known conditions. The microstructures observed in the experimental samples have provided a valuable foundation for the interpretation of similar microstructures in the natural samples. The most important aspect of our experimental study, however, has been the examination of permanent deformation in single crystals before macroscopic strain is observed.

Progress

Our experiments of one week to one month duration produced permanent heterogeneous deformation in thick-

walled hollow cylinders of single crystals of calcite. We chose the cylindrical shape for the simplicity of the stress gradient produced under our experimental conditions. We realized, however, that the duration of an experimental run should be extended if we were to observe evidence of dissolution, and we therefore initiated a seven-month run. The marked contrast between the microstructures observed in these experimental samples suggested that we had experimentally obtained microstructures associated with dissolution. Comparison of the location of these microstructures to the location of permanent deformation in the shorter-duration samples suggested that the dissolution-related microstructures had replaced the permanent deformation microstructures. The evidence of permanent strain-enhanced dissolution in the experimental samples has been used to support a similar argument based on comparable microstructures in the natural limestone samples.

The stress concentrations calculated for the samples did not exceed the experimentally determined critical resolved shear stress (CRSS); the calculated effect of twinning back stresses did not reinforce the observed dislocation activation. Therefore, we could not explain the observed dislocation activation in terms of stress concentrations exceeding the CRSS. The sensitivity of the volumeters used in our experiments had assured us that no dilation greater than 0.04% had occurred in any of our samples. The experimentally determined CRSS (based on macroscopic strain) is possibly not an appropriate parameter to predict dislocation activation.

During the past year, we conducted experiments to bracket the threshold stress of dislocation activation. Tetragonal calcite specimens (shape chosen to minimize the stress gradient) were subjected to stresses 50, 60, and 70% of the macroscopic yield stress at room temperature and 5 kbar confining pressure. Preliminary TEM observations of dislocations activated in the sample stressed at 50% of the yield stress supported the conclusions obtained from the original stress-gradient experiments.

Annemarie Meike (1986), Ph.D. Thesis, Department of Geology and Geophysics, University of California, Berkeley.

Reference

Conductivity of Mantle Rocks Between 20 and 600°C

Principal Investigator: S. Constable (UC San Diego)
LLNL Collaborator: A. G. Duba

Abstract

We are undertaking laboratory studies of the electrical conductivity of representative upper-mantle rocks in the temperature range from 20 to 600 °C. The results of our laboratory work will assist in the interpretation of the sea floor electromagnetic sounding data currently being collected at the Scripps Institution of Oceanography, UC San Diego. Data from previous studies of single-crystal olivine conductivity at upper-mantle temperatures have already proved important in interpreting the sounding data. We intend to extend single-crystal olivine data to whole-rock measurements in a temperature range relevant to the subcrustal oceanic lithosphere; sea-floor electrical sounding studies show this to have a low conductivity of 10^{-5} S/m or less. This value is still too high, however, to be explained by mineral conduction; we hope to determine whether grain boundary impurities lower the resistivity of dry rock to the value measured, or whether small quantities of free water are required.

Objectives

Although laboratory conductivity studies on single crystals of olivine have greatly assisted our understanding of the mantle conductivity structure, the effects of grain boundaries and impurities present in whole rocks is not well understood. Measurements of whole rocks in the laboratory at elevated temperatures are difficult because of the extremely long times required to reach kinetic equilibrium, and by thermally driven cracking, resulting in loss of grain-to-grain contact. By making measurements at lower temperatures, the problems of grain cohesion and equilibration of the conduction mechanism may be avoided, and we can address two important problems—we can determine the importance of the effect of conduction along grain boundaries, and whether the sea-floor electrical sounding data collected by Cox et al. (1985) require the presence of free water in the sub-crustal lithosphere.

We prepared six 1-mm-thick specimens of dunite—a rock composed of pure olivine—for study. We chose dunite because the behavior of its individual crystals can be predicted and used to assess the extent of grain-boundary conduction. Conductivity will be measured up to 600°C at LLNL, and scanning electron microscopy will be performed at UC San Diego on both heated and unheated specimens.

Progress

X-ray dispersion in a scanning electron microscope was used to determine that these specimens have a Mg/Fe ratio of 5–8. This result will permit relating the conduction data to previous data for single-crystal olivine with a Mg/Fe ratio of 5.

Cox, C. S., S. C. Constable, A. D. Chave, and S. C. Webb (1986), "Controlled Source Electromagnetic Sounding of the Ocean Lithosphere," *Nature*, **320**, pp. 52-54.

Reference

Measurement of the Hall Effect in Olivine at High Temperature

Principal Investigator: C-Y Wang (UC Berkeley)

LLNL Collaborator: A. G. Duba

UC Berkeley Student: L. Hirsch

Abstract

We sought to measure the Hall effect and the electrical conductivity of single crystals of San Carlos olivine subjected to temperatures to 1500 K and to oxygen fugacities within the olivine stability field. From these data, we can derive the sign of the charge carriers and their mobility, as well as their concentrations. We calculated that the electromotive force resulting from the Hall effect in olivine is likely to be small, and we have spent much effort in attempting to reduce the ambient electrical noise in our high-temperature apparatus. Unfortunately, due to our current experimental configuration, we believe we cannot sufficiently reduce the level of noise without extensive expenditure of both time and funds.

Objectives

The motion of point defects in mantle minerals controls many of the physical and chemical properties in the mantle; however, a detailed knowledge of the generation and motion of these defects is lacking. Measurements of the Hall effect (the development of a transverse electric field when a conductor is placed in a magnetic field) and the electrical conductivity, along with application of defect chemistry theory, serve as an effective means to identify the predominant defects and their transport characteristics. However, Hall effect measurements have not been performed on mantle minerals at temperatures appropriate to the mantle (~1500 K). We are attempting to measure the Hall effect in San Carlos olivine in order to better understand the mechanisms of electrical conduction and solid-state deformation in the Earth's upper mantle. We also hope to introduce Hall-effect measurement techniques as a useful tool for attaining important information on the properties of point defects in other mantle minerals.

In order to perform this measurement, we had to overcome two major technical problems. The first was to locate a solenoid magnet with a sufficiently large field intensity and a large enough central bore to accommodate our high-temperature furnace. In general, the few compatible magnets we found at LLNL, Lawrence Berkeley Laboratory, and UC Berkeley would have required a prohibitively long period of time and expense to restore them to good operating condition. Another difficulty was that many superconducting magnets employ liquid helium within their central bore and thus could not accommodate our furnace. We finally located a 14-cm bore, 12.5 Tesla magnet at the Francis Bitter National Magnet Lab at the Massachusetts Institute of Technology, which we could use at a relatively low cost.

We also modified an existing high-temperature electrical-conductivity apparatus to perform the Hall effect measurements. Three main issues were associated with this modification: since we did not know the Hall electromotive force (EMF) generated from the alumina ceramics in our furnace itself under our experimental conditions, we had to carefully construct a sample holder that did not have a spurious conduction path through alumina. After considering several designs, we chose to employ a cylindrical alumina tube in which a disk-shaped olivine specimen could be held; longitudinal slits in the tube largely prevent conduction through the holder.

Another issue for Hall effect measurements of high-resistance materials is that a substantial EMF may exist across the voltage leads. This can result from not placing the voltage leads in a perfectly symmetric orientation with respect to the current leads, or from minor sample inhomogeneities. Since this misalignment voltage can be orders of magnitude larger than the actual Hall EMF, an external compensation circuit had to be constructed to nullify this effect. Although we tried an extensive number of different standard designs for this circuit, we could not nullify this noise to a level sufficiently low to justify the Hall effect measurements. At present, we believe the best solution would be to construct a new apparatus. We are now in the design stage, and we are determining the feasibility of this apparatus.

References

Hirsch, L. M., and C. Y. Wang (1986), "Carrier Mobility in the Presence of Dislocations?" *Geophys. Res. Lett.*, **13**, pp. 487-490.

Hirsch, L. M. and C. Y. Wang (1986), "Electrical Conductivity of Olivine During High-Temperature Creep," *J. Geophys. Res.* **91**, pp. 10,429-10,441.

Dynamic High-Pressure Processing and Synthesis of Novel Materials

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

LLNL Collaborator: W. J. Nellis

UC San Diego Student: J. Neumeier

UC San Diego Postdoctoral Researcher: M. Torikachvili

We are synthesizing new metastable materials with novel crystalline and microstructures. Specimens are subjected to megabar shock pressures and temperatures of several thousand degrees Kelvin; these specimens are recovered intact at the LLNL two-stage light-gas gun, and sent to UC San Diego for investigation. The shock process creates temperature and pressure quench rates that are sufficiently fast to produce metastable structures—structures frozen in from the extreme formation conditions, such as cannot be created by conventional processing techniques. Our goal is to synthesize superconducting and magnetic materials with performance characteristics substantially superior to those available at present.

Abstract

We are attempting to produce novel materials by processing specimens at megabar dynamic pressures, and several-thousand-degree Kelvin temperatures. Our goal is to synthesize metastable solid phases of potentially high- T_c superconductors, ultrahigh-critical-magnetic-field (H_c) superconductors, and ultra-hard permanent magnets by shock-induced crystal and/or microstructure. We feel these goals are feasible because of the high densities and temperatures used to drive phase transitions and the high calculated quench rates from extreme conditions: 10^9 K/s in solid specimens, 10^6 – 10^8 K/s in initially powder specimens, and 10^{12} bar/s in all specimens.

Objectives

We previously developed a shock-recovery fixture that enabled specimens to be recovered from pressures in the range 0.6–1.2 Mbar. We have refined this recovery fixture to a modular design with cryogenic precooling. The modular design enables the cryogenic chill block to be

Progress

reused even when the specimen has been shocked to a megabar. Precooling maximizes quench rates and, thus, the retention of metastable phases. We also refined our projectile design, so that our 5–10 g projectile can process a specimen of Nb_3Si three times larger than had been investigated previously using 1000 g of explosives. Also, the fixture was adapted to allow powdered specimens to be shock melted and thermally quenched in a copper matrix. We are currently preparing a patent application for shock synthesis.

Last year, we showed that the superconducting transition temperature T_c of Nb is only weakly sensitive to Mbar dynamic pressures. Our recent results reveal that the upper critical magnetic field H_c is enhanced by a factor of two, probably caused by shock-induced defects predicted to have a maximum concentration in Nb shocked to about 0.9 Mbar.

Two arc-melted bulk specimens of Nb_3Si were shocked to pressures in the megabar range. Our calculated dynamic pressures, temperatures, and densities increase to their peak magnitudes in nanosecond time scales, plateau for several hundred nanoseconds, and decay in a comparable time. The thermal quench of a solid has a fast thermodynamic cooling rate of 10^9 K/s for the first few hundred K drop below maximum temperatures of 1000–2000 K, followed by slower cooling by thermal diffusion. This history is appropriate for synthesizing phases induced at peak pressure and cooled sufficiently and quickly during the first stage to remain metastable during the slower second-stage cooling. The Nb_3Si sample shocked to 0.96 Mbar shows an onset of T_c at 18 K by a sharp drop to zero of the electrical resistance, as is illustrated in the Figure. Previous attempts by other researchers to prepare the A15 phase of Nb_3Si by shock compression yielded only a weak inflection in resistance at 18 K. Our x-ray data show peaks for the A15 phase of Nb_3Si that correspond to a lattice parameter of 5.09 Å and significant portions of other phases. The x-ray data also shows that the superconducting A15 phase is synthesized at the expense of Ti_3P -type phase in the starting specimens. The Ti_3P phase is a high-temperature metastable phase that can be made by conventional techniques. Specimens richer in the Ti_3P phase will be prepared to optimize the conver-

sion to the shock-synthesized Al₅ structure and to achieve higher values of T_c and H_c .

We prepared specimens of $PbMo_6S_8$ by powder metallurgical techniques, and then designed dynamic pressure experiments to shock melt and quench powder specimens. We hope to synthesize fine-grained specimens to enhance H_c , which is already the highest value (~60 T) ever reported for any material.

References

Nellis, W. J., M. B. Maple, and T. H. Geballe (1986), "Synthesis of Metastable Materials by High Dynamic Pressures," submitted to the Materials Research Society for Communications on the Materials Science and Engineering Study; selected for presentation at the 1986 MRS Fall Meeting.

Neumeier, J. J., M. S. Torikachvili, M. B. Maple, W. J. Nellis, and H. B. Radousky (1986), "Superconducting Properties of Nb and Nb Compounds Recovered from Megabar Dynamic Pressure," *Bull. Am. Phys. Soc.*, **31**, p. 640.

Nellis, W. J., W. C. Moss, H. B. Radousky, A. C. Mitchell, L. T. Summers, E. N. Dalder, M. B. Maple, and M. McElfresh (1985), "Superconducting Critical Temperatures of Niobium Recovered from Megabar Dynamic Pressures," *Physica*, **135B**, p. 240.

Nellis, W. J., W. C. Moss, H. B. Radousky, A. C. Mitchell, L. T. Summers, E. N. Dalder, M. B. Maple, and M. McElfresh (1986), *Shock Waves in Condensed Matter*, Y. M. Gupta, Ed. (Plenum, New York), p. 719.

The ratio of specimen resistance to its resistance at 300 K vs temperature. The lower-temperature transition at 9 K is caused by a partial amount of disordered Nb-Si alloy in the starting specimens. The transition at 18 K is caused by the shock-synthesized A15 phase. A shock pressure of 0.96 Mbar caused the electrical resistance to go to zero at 18 K. A shock pressure of 0.82 Mbar induces the A15 phase but not enough to cause zero resistance.

Astrophysics Research Center

Nuclear Astrophysics and Radiation Transport

Principal Investigator: S. E. Woosley (UC Santa Cruz)
LLNL Collaborators: T. Axelrod, R. Klein, and T. Weaver
UC Santa Cruz Students: D. Hartmann and P. Pinto
Other Collaborators: J. Arons (UC Berkeley)

In a number of computationally intensive problems, we are investigating the nature of Type I and II supernovae. These problems include the mechanisms of thermonuclear deflagration and gravitational collapse in a supernova; the nucleosynthesis produced by high-temperature nuclear reactions; and the light curve and spectra, especially of Type I supernovae. Our results provide a quantitative framework for the classification and physical interpretation of supernovae. We are also using this expertise to study other high-energy phenomena, such as cosmic gamma-ray bursts, and particularly the "optical flashes" that have allegedly accompanied such bursts.

Abstract

We are attempting to provide a quantitative framework for the classification of and physical interpretation of supernovae. To accomplish this, we are performing hydrodynamic modelling of supernova explosions and studying radiative transfer in extremely hot, expanding clouds of gas. We are also using this expertise to study other high-energy phenomena, such as cosmic gamma-ray bursts, including the "optical flashes" that have allegedly accompanied such bursts.

Objectives

One interesting outcome of this study has been a new model for Type Ib supernovae that represents a reasonable alternative to the scenario frequently discussed in the recent literature: Wolf-Rayet explosion. While we are calculating light curves and spectra expected of Wolf-

Progress

Rayet star explosions, we have also considered the observational consequences of a deflagration that propagates through a portion of a carbon-oxygen white dwarf with a flame speed much slower than is usually employed in the standard models for Type Ia supernovae. If the turbulent flame speed is only a few hundred kilometers per second (still much faster than conduction, ~ 50 km/s), then the white dwarf may become entirely unbound, but still produce only a few tenths of a solar mass of iron and nickel. The lower explosion energy of a Type Ib supernova means a slower expansion, which, combined with the smaller amount of radioactivity, implies a broader, dimmer light curve. The small amount of radioactivity and the large amount of unburned oxygen in the outer layers have also been shown by Pinto and Axelrod to give a late time spectrum dominated by emission lines of neutral oxygen, similar in many respects to what is seen in Type Ib spectra taken at peak light. If this model is the correct explanation of Type Ib supernovae, then such supernovae may eventually be observed in elliptical galaxies, although the few representative examples have thus far all been in spirals.

References

- Woosley, S.E., and T.A. Weaver (1987), "The Explosion of a Wolf-Rayet Star I: Dynamics and Nucleosynthesis," to be submitted to *Ap. J.*
- Ensman, L., and S.E. Woosley (1987), "The Explosion of a Wolf-Rayet Star II: Light Curves," to be submitted to *Ap. J.*
- Axelrod, T., P. Pinto, and S.E. Woosley (1987), "The Explosion of a Wolf-Rayet Star III: Late Time Spectra," to be submitted to *Ap. J.*

Gravitational Perturbations in Spiral and Elliptical Galaxies

Principal Investigator: L. Hernquist (UC Berkeley)

LLNL Collaborator: C. E. Max

UC Berkeley Collaborator: D. Merritt (now at University of Toronto)

Other Collaborator: P. J. Quinn (California Institute of Technology and Space Telescope Science Institute)

With computer models, we are using gravitational N-body techniques to study the effects of gravitational perturbations on the dynamics and stability of spiral and elliptical galaxies. In particular, we have investigated the possible influence of satellite galaxies on the evolution and characteristics of spiral galaxies. Our initial tests, performed on the LLNL National Magnetic Fusion Energy Computer Center's Cray X-MP and Cray-2 computers, indicate that mergers even with low-mass satellites (~1% of the mass of the spiral) can heat galactic disks efficiently and can result in an observable increase in the scale-height perpendicular to the disk plane. We are attempting to use these simulations to place constraints on the amount of material that typical galaxies may have accreted during the Hubble time—this information will be directly relevant to theories of galaxy formation. We are also studying the applicability of various N-body algorithms to more subtle aspects of galactic dynamics.

Abstract

Recent studies have suggested that the evolution of galaxies may be significantly modified by small gravitational perturbations. For instance, some observations indicate that galactic activity and the onset of enhanced star formation may be correlated with the presence of interacting companions. In addition, it has been known for some time that mergers of galaxies with low-mass satellites are responsible for a variety of effects, such as changes in morphology and the deposition of gas and dust in otherwise barren systems. Intrinsic non-uniformities in the potential wells of galaxies may themselves provide sources of gravitational energy for driving global instabilities in both spiral and elliptical galaxies. Previous studies

Objectives

have suggested that rotating bars in spiral galaxies are efficient in transferring gas from disks to bulges, thereby providing fuel for nuclear activity. Due to the non-linear nature of these phenomena, numerical methods and models are required to give insight into these processes. The goal of our project has been to use computational N-body methods to study the relevance of gravitational perturbations to the evolution and formation of galaxies.

Progress

Initially, we attempted to determine the most appropriate N-body algorithms for the effects we wished to investigate. Some problems, such as the sinking of satellites around spiral galaxies, do not pose severe difficulties for conventional N-body techniques; however, more subtle studies, such as the coupling between interacting companions and activity in the nuclei of spirals, cannot be so easily addressed. For example, understanding the propagation of density waves near the central regions of spiral galaxies requires a much higher spatial resolution than can be achieved with Eulerian codes. This led us to consider alternative approaches.

As a first step, we began to study the effect of mergers on spirals using a Caltech particle-mesh code. Previous work on this problem ignored the self-gravity of the disks and focused solely on the exchange of energy between the satellite and stars in the disk. Consequently, it had not been possible to obtain highly accurate estimates for the sinking rates of satellites around spirals or to determine the self-consistent response of the disk to the merger. Our initial simulations, performed on the Cray-2 with $N = 32,768$ particles, indicate that the previous calculations may have underestimated the sinking rates by factors of three for satellites within the disk planes, and by factors of four for satellites with orbits primarily outside the disks. In addition, satellites in orbits inclined with respect to the disk plane can efficiently transfer energy into the z-motions of the disk stars themselves. Disk scale heights can be increased by factors of two to three on a timescale comparable to the orbital time of the satellite. If these conclusions are verified, they will place severe constraints on the phase-space density of allowed satellite orbits to remain consistent with observations. For example, inclined orbits with radii less than or com-

parable to the disk radius will be forbidden if spiral galaxies must remain sufficiently thin for a Hubble time. Furthermore, satellite accretions may be much rarer events than has been previously thought. Such considerations may provide important clues for the formation of galaxies and galaxy/satellite complexes.

In addition to continuing our parameter study of sinking satellite effects, we have begun to investigate the forcing of spiral density waves in disks by orbiting companions. Initial tests with Hernquist's new "tree" code indicate that since the spatial resolution of this method is not limited by the presence of a fixed grid, it will be possible to follow the propagation of density waves near the central regions of spiral galaxies. In particular, we plan to analyze the structure of the resonances near the inner edges of realistic disks. If the waves can be transmitted through these resonances, it may be possible to couple interacting companions with the nucleus through the stellar component of disks alone. If this process is not efficient, then it will be necessary to include the gaseous component if stellar dynamical processes are to account for Seyfert activity. Our next step will be to merge the tree code with Quinn's sticky-particle code to provide a heuristic description of the response of the gas. Such a refinement will also enable us to determine whether or not density waves can account for recent IRAS observations that suggest higher rates of star formation in galaxies with interacting companions.

Hernquist, Lars (1987), *Performance Characteristics of Tree Codes*, Lawrence Livermore National Laboratory, Livermore, CA UCRL-95929.

Reference

Computer simulation of the orbital decay of a small satellite galaxy (black circle) in a direct coplanar orbit around a larger disk galaxy. Time is measured in units of 10^6 years, and each frame is 60 kpc across. When the orbit of the satellite is inclined to the plane of the disk galaxy, significant heating of the disk in the vertical direction results from the encounter.

Laboratory Studies in X-Ray Transfer Physics Relevant to Cosmic Sources

Principal Investigator: S. M. Kahn (UC Berkeley)

LLNL Collaborator: R. Lee

Campus Co-Experimenters: R. W. Falcone (UC Berkeley), M. Hettrick (LBL)

LLNL Co-Experimenters: R. London and G. Kolbe

UC Berkeley Students: W. Craig and J. Schachter

Abstract

We are investigating the practicality of conducting laser plasma experiments in the laboratory to study the physics of cosmic x-ray transfer processes. These transfer processes are believed to occur in many cosmic sources, particularly those involving x-ray photoionized nebulae (e.g., cataclysmic variables, x-ray binaries, and active galactic nuclei). Laser plasmas share a number of similarities to such sources, making small-scale laboratory experiments attractive and convenient to study these phenomena. We have concentrated our efforts on developing the instrumentation and analytical resources necessary to construct two specific experiments: a laboratory demonstration of the "Bowen fluorescence" mechanism that involves optical pumping associated with a wavelength coincidence between resonance transitions of He II, O III, and N III; and a measurement of the K-shell and L-shell photoabsorption cross sections of intermediate ions of carbon, and possibly of nitrogen and oxygen. We have designed, constructed, and tested a novel short-wavelength grazing-incidence reflection grating spectrometer, coupled to a streak camera to provide time-resolved measurements. The actual laser experiments are being carried out at the Janus Research Laser Facility at LLNL and at an additional desktop laser plasma facility on the UC Berkeley campus.

Objectives

Moderate- to high-resolution spectroscopy of cosmic sources at extreme ultraviolet and soft x-ray energies is one of the most promising and exciting frontiers of astrophysical research. At present, little observational work exists in this area because of the limiting sensitivity of most previous space experiments. However, space obser-

vatory instruments currently under development will extend this field considerably within the next decade. The ability to analyze such spectroscopic measurements depends not only on the quality of the data, but also on our knowledge of basic atomic physics and radiation-transfer processes that are important in shaping the spectrum. Uncertainties in this latter area will limit our understanding of a large class of astrophysical investigations: those involving accretion-powered sources in which short-wavelength spectral features are formed in a large photoionized medium surrounding an intense central continuum x-ray source. In such an environment, the emitting gas is significantly overionized (relative to the electron temperature), so that excited level populations are determined largely by recombination and photoexcitation, rather than by collisional excitation. The medium is also usually optically thick to important resonance transitions, so line-transfer effects are important. Since laser plasmas enter a similar state during the intermediate stages of their evolution, laser plasma research presents a promising alternative to study these phenomena. The experiments we are developing are of intrinsic interest in that they address specific issues necessary to the interpretation of existing data; in addition, these experiments are "representative," and were designed to exemplify the general usefulness of this type of research.

Progress

In the past year, we have designed and constructed a short-wavelength spectrometer that is especially well suited to making the time-resolved spectral measurements crucial to these experiments. We have also performed several analytical and numerical calculations to evaluate the feasibility of simulating the appropriate astrophysical conditions. The spectrometer is of novel design, developed specifically for these experiments. It incorporates a varied-line-space reflection grating that can provide high-resolution extreme-ultraviolet and x-ray spectra imaged on a focal plane at normal incidence to the beam. At the back, a soft x-ray streak camera displaces the spectrum as a function of time (with a time resolution of 0.1 ns), thereby yielding a two-dimensional image, which is displayed optically on a phosphor screen. We also incorporate a charge-coupled device (CCD) camera behind the streak camera to read the optical image and

compile a digital time-resolved spectrum. Our initial tests of the system used film to image the spectrum in place of the streak camera and CCD. The actual spectrum shows almost no astigmatism in the direction perpendicular to the dispersion, which implies that all the light intercepted by the grating does indeed get focused onto the streak-camera slit. The Figure shows a microdensitometer trace of a spectrum obtained with a carbon target; we have identified the prominent lines. The spectral resolution achieved is ~ 200 in the soft x-ray band (10–50 Å), which is far superior to that of competing technologies. Our resolution is in fact limited by the spatial extent of the plasma, so that higher resolution can in principle be obtained if we incorporate a slit in the system.

Our calculational work has focused on the feasibility of performing photoabsorption experiments using carbon as a target. We use two laser plasmas, one to produce the background continuum radiation and one to serve as the target ionized plasma for the absorption experiment. It is essential in such a configuration that the background continuum dominate the continuum and line radiation from the target plasma. This probably can be accomplished by introducing a time delay between the two pulses. Since the recombination time scale should be much slower than the cooling time scale, the target plasma should remain ionized after it has cooled. If the continuum-producing pulse occurs during this cool recombination-dominated phase, then the target plasma can be observed cleanly in absorption. We have used a 1-D version of the LASNEX code at LLNL to calculate the hydrodynamics and radiation transport within the absorbing plasma, and the XRASER code to find the detailed ionization structure. Both solid cylinder and thin foil CH targets were considered. The thin foils appear to be preferable, since at intensities appropriate for producing He-like ions, the laser may burn through, producing a central region that is relatively free of steep gradients in temperature and density. To get to lower ionization stages, a lower intensity is required; it may be more difficult for the laser to burn through unless thinner foils can be fabricated.

The principal question we wanted to evaluate for this experiment involves the practicality of obtaining significant optical depth in the photoelectric continuum of

any particular ion. As discussed above, one must wait until the absorbing plasma enters the recombination phase in order to suppress its emission. However, during this time interval, the plasma also expands, thereby decreasing its central density. We find that the characteristic cooling time for the carbon plasma is 5 ns for appropriate laser parameters. After this amount of time, the central density drops to $10^{19}/\text{cm}^3$. The cross-section at the K-edge for these carbon ions should be a few $\times 10^{-19} \text{ cm}^2$, so an optical depth of unity requires a path length of several millimeters. Hence, it will be necessary to use a line focus for the absorbing plasma target. The calculations suggest that the experiment will be challenging, but feasible. Experimental tests at Janus have recently begun.

References

Hettrick, M.C. (1987), "High-Resolution Gratings for the Soft X Ray: Aberration Correction Methods and Their Performance Limitations," submitted to *Nucl. Instruments and Methods*.

Kahn, S.M., W. Craig, R.W. Falcone, M.C. Hettrick, and J. Schachter (1987), "Varied Line Spacing Grating for X-Ray Transfer Experiments in Optically Thick Plasmas," to be submitted to *Applied Optics*.

A microdensitometer trace of a soft x-ray/extreme ultraviolet spectrum of a carbon plasma recorded on Kodak 101 x-ray sensitive film and obtained with the grazing-incidence short-wavelength spectrometer developed in connection with this program. The prominent lines are identified. The spectrometer has appreciable sensitivity down to wavelengths as short as 30 Å, and note the absence of astigmatism in the image. The spectral lines are mostly from H-like and He-like carbon.

The Emission Lines from Quasars and Seyfert Galaxies

Principal Investigator: R. C. Puetter (UC San Diego)

LLNL Collaborators: G. Fisher and S. Langer

UC San Diego Student: I. Krinsky

Abstract

Some researchers have proposed the existence of a confining, hot (10^8K) medium surrounding the cold (10^4K) broad-line clouds in quasars and Seyfert galaxies. We are modifying an existing radiative hydrodynamics computer code used for modeling solar flares so that it can handle the physical conditions appropriate to the interface region between these cold and hot media. The modified computer code will allow us to model these objects and investigate a number of pertinent facts concerning cloud properties. With the new code, we can better understand cloud stability and breakup modes, the nature of evaporative winds from the broad-line clouds, and the extent of line and continuum emission from the hot/cold interface region. We have made significant progress in modifying the code, and we expect concrete scientific results shortly.

Objectives

Our goal is to achieve a better understanding of the properties of the broad-line clouds that are observed in the spectra of quasars and Seyfert galaxies. Such dense, low-mass clouds are apparently moving at high velocities and would dissipate rapidly (within one year) due to free expansion if they were not confined by some mechanism. For this reason, some researchers have proposed that a second hot phase of roughly equal gas pressure exists in thermodynamic equilibrium with the cool broad-line clouds. Such an intercloud medium should stabilize the broad-line clouds and preserve them over the dynamical time scale of the broad-line region ($100\text{ years} \approx \text{broad-line region cloud crossing time}$). Preliminary studies of cloud evaporation and conductive fluxes through the cloud boundary in the presence of an intercloud medium have already been made, but these have fallen short of a detailed dynamical study of cloud breakup due to instabilities or any study of the line and continuum fluxes arising from the interface zone. Such considerations alone could

have profound implications for broad-line cloud physics and might even rule out a confining intercloud medium scenario.

Progress

We have begun modifications to an existing radiative hydrodynamics code running on the LLNL Magnetic Fusion Energy Computer Center Cray computers. The original code has been used to model solar flare loops, but modest changes must be made before we can use it to model quasar and Seyfert broad-line cloud/hot medium interfaces. The first significant change must be made to the boundary conditions—the solar flare loop calculation uses a semi-infinite geometry, but the quasar cloud problem requires a finite slab geometry. A second change involves the inclusion of ultraviolet to soft x-ray photoionization in the quasar cloud case: while this is unimportant and ignored in solar flares, this dominates the energetics of the gas in the quasar and Seyfert case. Another modification to the code involves the pertinent temperature ranges and appropriate physical processes, which encompass 10^8 – 10^4 K in the quasar case, but only 10^6 K to roughly 10^4 K in the solar flare case.

We have already incorporated most of these changes; however, after attempting to run the code, computational difficulties pointed up yet another change that must be made before a converged solution can be obtained. To make each of these problems (solar flare and quasar cloud) computationally tractable, we adopted an approximate radiative-transfer technique (i.e., first-order radiative transfer). For the solar flare case, we successfully used a single-stream approach. We have now learned, though, that in order to accurately follow the “back-heating” of the intercloud medium at both the front and back cloud boundaries, a two-stream technique must be used for quasars, allowing us to set radiative boundary conditions at each surface. This involves a considerable, but still tractable, modification to the existing program. We have resolved this problem, and we are near to completing the code modifications.

Balbus, S. A., and C. F. McKee (1982), "The Evaporation of Spherical Clouds in a Hot Gas II: Suprathermal Evaporation," *Ap. J.*, **252**, p. 529

References

Cowie, L. L., and C. F. McKee (1977), "The Evaporation of Spherical Clouds in a Hot Gas I: Classical and Saturated Mass Loss Rates," *Ap. J.*, **211**, p. 135.

Krolik, J. H., C. F. McKee, and C. B. Tarter (1981), "Two-Phase Models of Quasar Emission Line Regions," *Ap. J.*, **249**, p. 422.

McKee, C. F., and L.L. Cowie (1977), "The Evaporation of Spherical Clouds II: Effects of Radiation," *Ap. J.*, **215**, p. 213.

Dynamics and X-Ray Spectra of Inhomogeneous Young Supernova Remnants

Principal Investigator: C. F. McKee (UC Berkeley)

LLNL Collaborator: C. B. Tarter

UC Berkeley Student: C. J. Romanik

Abstract

With the aim of modeling the emission and structure of young supernova remnants, we are compiling atomic data and carrying out a calculation of the dielectronic recombination rate. We have nearly completed our calculation of the dielectronic recombination rate coefficients for all astrophysically abundant ions. Our results have shown that large errors exist in the rate coefficients currently used in calculations of the ionization states of ions in astrophysical plasmas. Our improved set of data will be useful for these and other problems where such recombination is important.

Objectives

X-ray observations of young supernova remnants show spatially inhomogeneous emission from many highly ionized elements. In attempting to infer the structure of the supernova remnant from this data, investigators have used spherically symmetric models of supernova remnants and used available atomic data to calculate the emission. The goal of our project is to explore the consequences of spatial inhomogeneities on the emission and evolution of the remnants, when conduction and evaporation may be important. As a result, we will be generating an improved set of atomic data for use in this and similar problems.

Progress

We have made calculations of dielectronic recombination rates for ions of the He, Li, Be, and the Ne isoelectronic sequences. Our results have shown that large errors are present in many of the rates used in current astrophysical calculations. Ionization equilibrium calculations using our new ionization rates indicates that previous calculations of the temperature of maximum abundance of a particular ion may be in error by more than a factor of two. While our method of calculating the dielec-

tronic recombination rate makes many simplifying assumptions, we arrive at results that agree within a factor of two with the most detailed calculations that have been done. The relative simplicity of this method allows us to calculate the rates for all astrophysically abundant ions in a fairly straightforward manner, whereas more detailed calculations have been carried out for only a small number of ions. We plan to compute dielectronic recombination rates for more ions and use these to begin a sequence of model calculations of x-ray emission-line spectra from young supernova remnants.

Romanik, C. (1987), "Dielectronic Recombination Rates for Astrophysical Plasmas," submitted to *Ap. J.*

Reference

Computer Study of the Turbulent Mixing of Scalars

Principal Investigator: C. H. Gibson (UC San Diego)

LLNL Collaborator: R. M. Kerr

Other Collaborators: W. T. Ashurst and A. R. Kerstein
(Sandia National Laboratories, Livermore)

Abstract

Our understanding of many astrophysical processes that depend on turbulent mixing has been hindered by a poor knowledge of the fundamental small-scale mechanisms of turbulent mixing. Examples of such mechanisms include the turbulent mixing of strongly diffusive quantities, such as weakly-ionized plasmas that can affect electromagnetic wave scattering, or the mixing of magnetic fields by turbulence. The critical experiments necessary to distinguish between competing theories in this area are extremely difficult to do in the laboratory. Recent advances in numerical methods and in the speed and capacity of computers have finally given us the ability to perform some of the necessary experiments computationally. We have used three-dimensional computer simulations to explore the mechanism of turbulent diffusion in fluids and to compare the results with a variety of analytic theories for this process.

Objectives

We are investigating the mechanism of turbulent diffusion in fluids by means of computer simulation. Mechanisms of small-scale turbulent mixing will be studied using pseudo-spectral numerical methods in three dimensions. We will also explore more fully a consistent pattern in the spectral forms and correlation values determined both experimentally and by numerical simulations. Once the mechanisms of rate-of-strain mixing independent of Prandtl number are verified, we will use computer graphics to study the small-scale turbulent structures. Comparisons will be made with the predictions of Gibson (1968a,b) and Batchelor et al (1959).

Progress

Two very important results have emerged from statistical analysis of Kerr's previous turbulent mixing simulations (Kerr, 1985). Ashurst and Borgia were able

to recover results from the NASA/AMES computations reported by Kerr (1985); from this data, Ashurst computed the strain-rate/dissipation-rate correlation coefficient for turbulent mixing simulations with scalar Prandtl numbers of $Pr = 0.1, 0.5$, and 1.0 . All scalar fields mixed by turbulence show decorrelations of the strain-rate and dissipation-rate at the same separation distance r normalized by the Kolmogoroff scale L ; all are negatively correlated, with $\Sigma(0) \approx -0.5$ independent of Pr . This is precisely the result predicted by the mixing model and universal similarity hypotheses proposed by Gibson (1968a,b) and Gibson, Ashurst, and Kerstein (1985). However, this is inconsistent with the proposal of Batchelor et al. (1959) and others, that the mixing mechanism of turbulence depends on the diffusivity of the scalar field. The other major result has to do with the relative magnitude of the principal values of the rate-of-

$$\text{strain tensor } e_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right).$$

The principal axes of the tensor are chosen so that the $e_{11} = \alpha$ value is positive, $e_{22} = \beta$, and $e_{33} = \gamma$ is negative. From continuity, $\alpha + \beta + \gamma = 0$, so β may be either positive or negative.

It has long been a matter of curiosity (and of great practical interest in combustion theory) whether the average value of β is positive or negative. Four different hypotheses have been made, termed the "pasta" theories of turbulence by the late Les Kovasnay: the "ravioli" group expects fluid particles to be stretched in two directions and flattened in one, the "vermicelli" group favors distortion into ribbons, and the "spaghetti" group expects squashing in two directions and stretching of particles in one. Gibson (1968) shows that the Batchelor universal viscous-convective subrange constant β_b is bounded by

$\sqrt{3} \leq \beta_b \leq 2\sqrt{3}$ depending on $\bar{\beta}$. Because most laboratory and field measurements of β_b have been at the high end of the range, the "spaghetti" school has been favored. However, our analysis has shown the actual value of β/α is $+1/3$, with $\alpha : \beta : \gamma = 3 : 1 : -4$. Moreover, the locations of these flattening particles are in annular regions near vortex lines, as shown by the correlation $\langle \omega_i e_{ij} \omega_j \rangle = 2,538$

where $\beta > 0$, and is only 56 where $\beta < 0$. Therefore, on average, turbulent fluid particles appear to be twisting as well as flattening in two directions, perhaps giving rise to a new pasta school of turbulence ("rotelli?"). Clearly this also suggests that the reported measurements of β_β should be reexamined for possible errors that might produce a bias to larger values. A likely source for such errors is the intermittency of the normalizing dissipation rates, which is quite high for the high Reynolds-number field data, and which tends to increase estimates if it is not taken into account. Our new result would be virtually impossible to achieve without numerical simulation, and will have many practical consequences to the modeling of turbulent mixing, particularly in the field of combustion theory where "stretch" effects (due to the value of β / α) determine flame speeds and reaction rates.

References

- Batchelor, G. K., I. D. Howells, and A. A. Townsend (1959), "The Case of Large Conductivity: Part 1," *J. Fluid Mech.*, **5**, p. 134.
- Gibson, C. H. (1968a), "Fine Structure of Scalar Fields Mixed by Turbulence I: Zero-Gradient Points and Minimal Gradient Surfaces," *Phys. Fluids*, **11**, p. 2305.
- Gibson, C. H. (1968b), "Fine Structure of Scalar Fields Mixed by Turbulence II: Spectral Theory," *Phys. Fluids*, **11**, p. 2316.
- Gibson, C. H., W. T. Ashurst, and A. R. Kerstein (1985), "Mixing of Strongly Diffusive Passive Scalars Like Temperature by Turbulence," Sandia Report SAND84-8858 (to be published in *J. Fluid Mech.*).
- Kerr, R. M. (1985), "Kolmogoroff and Scalar Spectral Regimes in Numerical Turbulence," NASA Technical Memorandum, in preparation.

Plasma Astrophysics

Principal Investigator: J. Arons (UC Berkeley)

LLNL Collaborators: B. I. Cohen, R. I. Klein,

A. B. Langdon, C. E. Max

UC Berkeley Students: D. Burnard and A. Zachary

We studied the radiation gas dynamics of gravitational accretion flows onto the magnetic polar caps of strongly magnetized neutron stars. Our intent was to model the emission properties of accretion-powered x-ray pulsars, and we have obtained the first computational evidence for overstable convection in plasma over the polar caps of a neutron star. Our results suggest the presence of 10–100 ms fluctuations in the emergent spectra of these objects. In a separate project, we studied the diffusion of high-energy particles in the magnetized interstellar medium, in an effort to understand the basic physics of the acceleration of cosmic rays by interstellar shock waves. Using a novel plasma simulation code, we were able to study the diffusion of the particles in the magneto-hydrodynamic waves radiated by the particles themselves, as the particles drift at speeds above the Alfvén speed through the medium. When the drift speed is large, the wave amplitude is also large, leading to major modifications of the diffusion rates from those predicted analytically in the small amplitude regime.

Abstract

Accretion onto Neutron Stars

Our goal is to create self-consistent computational and analytic models of the velocity, temperature, and density structure of fully ionized plasma accreting along the polar field lines of a magnetized neutron star. Our models will be used to create synthetic spectra for comparison to the observed spectra of x-ray pulsars, which should tell us much about the physical conditions within the emission regions of these objects. Previous radiation-transfer models were constructed with single values of the plasma density and temperature, and have failed to give good representations of the detailed observed spectra, mainly because the radiation pressure observed requires drastic inhomogeneities in space and time. Our dynamical

Objectives

cal models under construction will provide the needed structures as functions of the (observable) luminosity of the systems.

Diffusion of Cosmic-Rays Near Shock Waves

The previous theory of cosmic-ray scattering by hydromagnetic waves assumes the wave amplitudes to be small. However, if interstellar shock waves are the sources of observed cosmic rays, then the hydromagnetic waves near each shock must have large amplitude in order to scatter particles back and forth across the shock many times. Our goal is to describe the generation of large-amplitude waves by streaming particles, and the scattering of particles by the waves, using the computational methods of plasma simulation; this "experiment" may reveal the physics of interaction in the large-amplitude regime.

Progress

Accretion onto Neutron Stars

We completed our study of the physical processes to be used in gas dynamical modeling, applying semi-classical models to derive computationally useful approximations to the physics, and also to derive a number of new results in the radiation transfer of polarized x-rays in the birefringent medium. We also made progress on our analytic solutions, which are useful in understanding the numerical results. Development of the computer code ACCRETE, which embodies all of the pertinent physical processes, approached its final state, with only the boundary conditions to be incorporated. During our developmental work, we found that the numerical solutions, which initially showed good agreement with the simplified analytical steady-flow models, develop large "photon bubbles" in the flow; the properties of these bubbles appear to be related to a form of convection in a strong magnetic field. We will attempt to follow the development of these bubbles for a sufficiently long time to see their predicted effects on time-resolved observations of the x rays from these systems.

Diffusion of Cosmic Rays Near Shock Waves

We have developed a new type of hybrid plasma-simulation code, in which Alfvén waves and the background interstellar medium are described as a one-dimen-

sional ideal magnetohydrodynamic fluid, while high-energy particles are modeled as a particle-in-cell plasma, whose net current gives their coupling to the Alfvén waves. Our code has been applied to the nonlinear saturation of the resonant-beam cyclotron instability, thought to be the dominant mechanism controlling the diffusion of high-energy particles near an interstellar shock wave as the particles undergo Fermi I acceleration. We find that the particles' pitch-angle diffusion is not well described by small-angle scattering when the waves saturate at the relevant large amplitudes. Instead the particles undergo occasional large jumps in pitch angle space, as shown in the Figure. These jumps appear to be due to resonance overlap in the multi-mode spectrum. In addition, we have studied the isotropization of an initially cold beam of particles, such as is observed ahead of the Earth's bow shock, in the necessarily long time limit. The result is a new, observationally testable proposal for the evolution of the velocity structure of particles observed in the interplanetary medium near the Earth.

References

- Arons, J. (1986), "Physics of Polar Cap Accretion onto Neutron Stars," *Plasma Penetration into Magnetospheres*, Proceedings of the Mediterranean School on Plasma Astrophysics, N. Kylafis, J. Papamastorakis, and J. Ventura, Eds. (Iraklion: Crete University Press), pp. 141–142.
- Arons, J., L. Hernquist, and R. I. Klein (1986), "Radiation Gas Dynamics and MHD Stability of Polar Cap Accretion onto Magnetized Neutron Stars," *Bull. Am. Phys. Soc.*, **31**, p. 811.
- Zachary, A., B. I. Cohen, C. M. Max, and J. Arons (1986), "Cosmic Ray Diffusion Ahead of a Supernova Remnant Shock Wave," *Bull. Am. Phys. Soc.*, **31**, p. 812.
- Arons, J. (1986), "Continuum Spectra from Polar Cap Accretion onto Magnetized Neutron Stars," a contribution to the chapter "Energy Sources" J. M. Hameury and J. P. Lasota, Eds. in *Proceedings of the Stanford Workshop 'Gamma Ray Bursts'*, E. Liang, and V. Petrosian, Eds. (American Institute of Physics, New York), pp. 168–174.

Arons, J., and J. J. Barnard (1986), "Wave Propagation in Pulsar Magnetospheres: Dispersion Relations and Normal Modes of Plasmas in Superstrong Magnetic Fields," *Ap. J.*, **302**, pp. 120–137.

Barnard, J.J., and J. Arons (1986), "Wave Propagation in Pulsar Magnetospheres: Refraction of Rays in the Open Flux Zone," *Ap. J.*, **302**, pp. 138–162.

Arons, J. (1986), "Centrifugally Driven Winds from X-Ray Pulsars," *Plasma Penetration into Magnetospheres*, Proceedings of the Mediterranean School on Plasma Astrophysics, N. Kylafis, J. Papamastorakis, and J. Ventura, Eds. (Iraklion: Crete University press), pp. 115–124.

Arons, J., R. I. Klein, and S. M. Lea (1987), "Radiation Gas Dynamics of Polar Cap Accretion onto Magnetized Neutron Stars: Basic Theory," *Ap. J.*, **312**, p. 666.

Arons, J. (1987), "Accretion onto Magnetized Neutron Stars: Polar Cap Flow and Centrifugally Driven Winds," *Origin and Evolution of Neutron Stars*, Proc. IAU Symp. No. 125, D. J. Helfand, Ed. (Reidel publishing co., Dordrecht, Netherlands), in press.

Arons, J., and R. I. Klein (1987), "Polar Cap Accretion onto Magnetized Neutron Stars: An Analytic Solution," *Origin and Evolution of Neutron Stars*, Proc. IAU Symp. No. 125, D. J. Helfand, Ed. (Reidel publishing co., Dordrecht, Netherlands), in press.

Klein, R.I., and J. Arons (1987), "Radiation Gas Dynamics of Polar Cap Accretion onto Magnetized Neutron Stars: Numerical Calculations," *Origin and Evolution of Neutron Stars*, Proceedings of IAU Symposium No. 125, D. J. Helfand, Ed. (Reidel publishing co., Dordrecht, Netherlands), in press.

Trajectories of three particles diffusing in large-amplitude hydromagnetic wave turbulence. The vertical axis is the cosine of the pitch angle of the particle's velocity vector relative to the magnetic field. The horizontal axis is the cyclotron frequency Ω times the elapsed time T . The top frame shows the adiabatic bounce-like motion of a particle that is not resonant with any hydromagnetic waves. The bottom two frames show the erratic diffusion of two resonant particles, both of which exhibit jumps in pitch angle on the order of 100% in 3–6 cyclotron periods.