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Section I. Overview

The Institute of Geophysics and Planetary Physics (IGPP) is a Multicampus Research Unit of the University of California (UC). IGPP was founded in 1946 at UC Los Angeles with a charter to further research in the earth and planetary sciences and in related fields. The Institute now has branches at UC campuses in Los Angeles, San Diego, Riverside, and most recently, Irvine and at Los Alamos and Lawrence Livermore national laboratories.

The University-wide IGPP has played an important role in establishing interdisciplinary research in the earth and planetary sciences. For example, IGPP was instrumental in founding the fields of physical oceanography and space physics, which at the time fell between the cracks of established university departments. Because of its multicampus orientation, IGPP has sponsored important interinstitutional consortia in the earth and planetary sciences. Each of the six branches has a somewhat different intellectual emphasis as a result of the strengths of campus departments and Laboratory programs.

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

IGPP-LLNL, like IGPP-Los Alamos, facilitates scientific collaborations between researchers at the UC campuses and those at the national laboratories in areas related to the earth sciences, planetary science, and astrophysics. It does this by sponsoring the University Collaborative Research Program (UCRP), which provides funds to UC campus scientists for joint research projects with LLNL. The goals of UCRP are to enrich research opportunities for UC campus scientists by making available to them some of LLNL's unique facilities and expertise and to broaden the scientific program at LLNL through collaborative or interdisciplinary work with UC campus researchers. UCRP funds (provided jointly by the Regents of the University of California and by the Director of LLNL) are awarded annually* on the basis of brief proposals, which are reviewed by a committee of scientists from UC campuses, LLNL programs, and external universities and research organizations. Typical funding for a collaborative research project ranges from \$5000 to \$25,000/year. Funds are used for various purposes, including to

*Further information about the University Collaborative Research Program, including guidelines for submitting proposals, may be obtained from Christina Budwine, Operations Manager, IGPP-LLNL, L-413, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551 (telephone: 510-423-4476; e-mail address: budwine@sunlight.llnl.gov).

support visiting graduate students, postdoctoral researchers, and faculty; experimental facility costs; released-time salaries for LLNL scientists; and the costs of supercomputing time.

Although the permanent LLNL staff assigned to IGPP is relatively small (about seven full-time equivalents), IGPP's research centers have become vital organizations. Each year, IGPP-LLNL supports a substantial group of resident postdoctoral fellows, funds 30 or more UCRP projects, and hosts a variety of visitors, guests, and faculty members on sabbatical leave, both from UC and other institutions. To focus attention on areas of interest in the geosciences and astrophysics, IGPP-LLNL also hosts conferences and workshops, and it organizes a seminar series for each research center: astrophysics, high-pressure sciences, and geosciences. Section IV lists the seminars given in FY 1992.

In FY 1992, 119 people were involved in 29 UCRP projects: 31 UC faculty members, 12 UC staff, 31 UC students, 42 LLNL investigators, and 3 scientists outside LLNL. Figure 1 shows the distribution of UCRP awards (previously called mini-grants) among the UC campuses by the total amount of funding and by the number of proposals funded. Table 1 lists the distribution of awards and the related

Figure 1.
Distribution of
FY 1992 awards to
UC campuses in
IGPP-LLNL's
University
Collaborative
Research Program:
(a) funds awarded
(in thousands of
dollars) and
(b) numbers of
awards. Northern
California campuses
received 49.6% of
the total funds
awarded; southern
California campuses
received 50.4%.

activity by each center within IGPP–LLNL. In addition, IGPP–LLNL hosted 26 outside scientists, who spent one week or more as residents at our main office at LLNL (Building 319).

Since FY 1987, IGPP–LLNL has maintained a bibliography of published research papers resulting from UCRP projects and from research by IGPP staff, postdoctoral researchers, and consultants. Section V gives the bibliography for FY 1992. Note that, because of the extensive peer-review process for most scientific journals, several papers submitted by the principal investigators are still in progress. Therefore, we cannot give an accurate total of 1992 papers published until we receive formal notification from the journals and authors. At present, we have published 62 papers in refereed journals or conference proceedings: 33 by UCRP researchers, 23 by IGPP researchers, and 6 by consultants. As a measure of research productivity, the results are gratifying. The abundance of publications from IGPP collaborative projects is a measure of the significance of the results obtained in these projects. The refereed-journal publication rate for FY 1992 IGPP-related projects corresponds to more than 1 paper/year for each UCRP faculty member, 2 papers/year for each IGPP postdoctoral researcher, and 2 papers/year for each IGPP staff member. Figure 2 compares the total papers published for the last three years.

Table 1. Distribution of UCRP awards and related activities for each IGPP research center at LLNL.

Research center	No. of projects	Funding (\$)	Supercomputing time (h)	No. of seminars
Astrophysics	8	184,750	88	61
Geosciences				21 ^a
Geochemistry	8	160,559	—	
Geophysics	5	102,240	21	
High-Pressure Sciences	8	141,059	155	22
Total	29	588,608	264	104

^aGeosciences seminars were supported jointly by IGPP–LLNL and LLNL's Earth Sciences Department.

To prepare for the future, IGPP-LLNL is exploring new directions in its research. These ventures, some of which are described in this report, include new applications of technologies developed for astrophysics experiments, research in geodesy, and our use of isotope analysis of rock samples to map tectonic movements over long periods.

Figure 2. Total number of IGPP-LLNL papers published in refereed journals and conference proceedings from 1990 through 1992. Note that, because of the extensive peer-review process for most scientific journals, several papers are still in progress. Therefore, we cannot give an accurate total of 1992 papers published until we receive formal notification from the journals and authors.

Section II. Highlights of Fiscal Year 1992

Center for High-Pressure Sciences

The Center for High-Pressure Sciences makes available LLNL's high-pressure experimental, theoretical, and computational modeling capabilities for collaborations between UC researchers and LLNL scientists. The collaborations include the use of experimental facilities and supercomputers at LLNL, joint theoretical research, and experimental work carried out at UC campuses on specimens that have been subjected to high pressures at LLNL. UC faculty, graduate students, and postdoctoral researchers participate in the program. Our high-pressure research encompasses geophysics, planetary physics, condensed-matter physics, chemistry, materials science, and engineering. LLNL researchers in high-pressure sciences are located in the Condensed Matter Physics (H) Division and in Earth Sciences. The Center Head is William Nellis, and Andrew Gratz is a postdoctoral fellow.

The principal facilities and capabilities at LLNL include

- *Two-stage light-gas guns* to measure equations of state; shock-wave profiles; electrical conductivities; and emission, Raman, and absorption spectra of minerals, liquids, and metals shocked to dynamic pressures of 100 GPa (1 Mbar) and temperatures of several thousand kelvins. We can also use gas guns to synthesize new materials by applying high dynamic pressures and temperatures followed by rapid quenching.
- *Diamond anvil cells* to measure equations of state up to 100 GPa by x-ray diffraction, laser heating, and Raman spectroscopy.
- *High-pressure systems* to determine stress-strain behavior, ultrasonic velocities, permeability, phase equilibria, fracture and flow properties, diffusion kinetics, and electrical and optical properties of minerals and ceramics up to 25 GPa and 2500°C.
- *Condensed-matter theory*, including electron-band theory of bulk and layered materials, fluid perturbation and mixture theories, Monte Carlo and molecular-dynamics methods, and dense-plasma theory.
- *Computational simulations* to study the performance of gas guns and the static high-pressure apparatus and the material response to dynamic loading.

Many of LLNL's high-pressure experimental facilities offer unique research opportunities. For example, the multianvil press and the two-stage gun are complementary methods for synthesizing and studying geologic and other materials. The multianvil press can subject specimens with volumes of 1 mm³ to pressures up to 25 GPa, temperatures up to 2500 K, and quench rates up to 100 K/s. The two-stage gun in specimens with volumes up to 1 cm³ achieves pressures up to 100 GPa, temperatures up to several thousand kelvins, and quench rates up to 10¹² bar/s and 10⁹ K/s. These two systems can synthesize a variety of high-pressure phases with a broad spectrum of microstructures and properties.

Unique facilities at LLNL and at Los Alamos National Laboratory can be integrated into one project. For example, Hans-Rudolph Wenk and Kristin Bennett of UC Berkeley and William Durham and Andrew Gratz of LLNL deformed ice specimens at LLNL's low-temperature static high-pressure facilities and two-stage gun. The crystallographic phases and textures induced were characterized by neutron diffraction spectroscopy at Los Alamos. The UC Berkeley research is supported by both IGPP-LLNL and IGPP-Los Alamos.

Research Highlights

Two-Stage Light-Gas Guns

Our 6.5-m-long, two-stage light-gas gun is located in an area of LLNL that is accessible to outside researchers without a security clearance. The gun has launch-tube diameters of 12, 20, and 35 mm, and the current maximum velocity is 4 km/s. We are implementing velocities up to 7 km/s with the 12-mm launch tube and hydrogen driving gas. We use a 19-m-long, two-stage light-gas gun and fast electronic, optical, and x-ray diagnostics to study planetary fluids. David Erskine is the technical supervisor of the gas guns, and Neal Hinsey is the operator of the 6.5-m-long gun.

Planetary Fluids

Shock compression of liquids produces high pressures and temperatures comparable to those in the giant planets Jupiter, Saturn, Uranus, and Neptune. The most abundant constituent of these planets and thus of the solar system is hydrogen. The external magnetic fields of Jupiter and Saturn, for example, arise from the convective flow of H_2 within their outer envelopes. To calculate the external magnetic fields, we must measure the electrical conductivities at relevant internal conditions. Therefore, Arthur Mitchell, Sam Weir, and William Nellis measured the electrical conductivities of liquid hydrogen that was shock-compressed by a single shock to pressures of 10 to 20 GPa (100 to 200 kbar), to temperatures of 3000 to 4500 K, and to threefold compression. The data yield a semiconducting electronic energy gap of 11.7 eV at 7.5 cm³/mol (Ref. 1), which agrees with recent theoretical calculations by Stephen Louie (UC Berkeley).

We are also measuring the electrical conductivities of liquid hydrogen shock-compressed with a shock wave reverberating between insulating anvils at pressures of 100 GPa and temperatures up to 4000 K. In these experiments, the temperature of hydrogen is low compared to the electronic bandgap. Preliminary results indicate that the conductivity curve from the 20-GPa experiments can be scaled to 100-GPa pressures and that the electronic bandgap of hydrogen predicted by UC Berkeley is followed reasonably well up to 100-GPa pressures for the disordered fluid, as in the giant planets. Also, the measured temperatures of hydrogen shocked up to 20 GPa agree with previous LLNL predictions.² Our electrical conductivity and shock temperature data are the only ones available for hydrogen at high pressures.

Impacts and Phase Transitions in Geologic Materials

Comets and asteroids colliding with planetary bodies generate high pressures and temperatures. The impact causes phenomena such as craters and produces materials with high-pressure phases and microstructures, such as amorphous quartz SiO_2 . Techniques have been developed to recover geologic materials from high dynamic pressures to investigate features such as phase transitions and microstructural changes.

To generate pressures in the 50-GPa range (10 to 500 kbar), we propel projectiles against planetary target specimens. The projectiles are accelerated with a 6.5-m-long, two-stage light-gas gun. The purpose of these experiments is to apply

high-impact shock pressures to the specimen, followed by very high quench rates to retain the phase and the microstructural features induced at high shock pressures. In this way, we can study the nature of the shock-induced phase and microstructural transitions in geologic materials in the laboratory and compare them with those found in nature.

For example, we shock-compressed cristobalite powder to very high pressures. Cristobalite has the same chemical formula as quartz, SiO_2 , which is the common form. Cristobalite is relatively rare and has a metastable high-temperature crystal structure that is different from the structure of quartz. Our results show that cristobalite transforms to the high-pressure amorphous form of SiO_2 at lower pressures and in a more narrow range of pressures than does quartz.³ In addition, the shock-induced microstructural features found in quartz⁴ are essentially absent in cristobalite. However, the high-pressure amorphous phases produced from both materials are essentially similar. Thus, the phase transformations in these two materials with the same chemical composition are quite different, although the final product phases are similar.³

The Cretaceous–Tertiary (K/T) boundary is a layer that is found essentially worldwide in the Earth. It contains a high concentration of quartz and feldspars with a distinctive microstructure similar to that found in these minerals when they are shocked to high pressures. This layer is thought to be the signature of a mass extinction of species, including the dinosaurs. The generally accepted cause of this layer is a hypervelocity impact caused by an asteroid colliding with the Earth. However, another proposal is that the K/T boundary was caused by explosive volcanism. To test the volcanism hypothesis, we performed novel experiments in which we applied pressure to granite in a way similar to that occurring in a volcano. The microstructural features in the recovered mineral specimens are dissimilar from those found in the K/T boundary layer. Thus, a giant impact, rather than a volcano, is the most probable cause of the K/T boundary.⁵

Astrophysics Research Center

The Astrophysics Research Center of IGPP-LLNL manages the astrophysics part of the UCRP and facilitates contacts between UC scientists and their LLNL counterparts. The Center also serves as the focus of astrophysics activities at LLNL by organizing the weekly astrophysics colloquium, hosting visitors and collaborators, and editing an annual observatory report, which covers all astrophysics activities at LLNL (and is published in the *Bulletin of the American Astronomical Society*). The Center provides a variety of other service functions, and the staff and postdoctoral researchers carry out a significant program of astrophysics research.

The scientific staff of the Astrophysics Research Center are Charles Alcock (Center Head), Claire Max, and Willem van Breugel. Administrative support is provided by Christina Budwine (Operations Manager) and by Arlene Manning and JoAnne McGuire (Administrative Specialists). Alan Edwards manages the network of computers. He is assisted by Deanne Proctor, who supports the astronomical image processing codes AIPS and IRAF, and by Susan Peterson, who is responsible for daily maintenance and for acquisitions.

Much of the research in the Astrophysics Research Center is carried out by the postdoctoral fellows, who have proved to be an energetic and stimulating group. Some fellows are supported entirely by IGPP funds, and others receive partial support from other groups at LLNL. In FY 1992, the postdoctoral fellows were David Bennett (previously at Princeton University), Leigh Brookshaw (Yale University), Susana Deustua (University of Michigan), George Hawkins (UC Los Angeles), Suzanne Hawley (Observatories of the Carnegie Institute of Washington), Scott Olivier (UC Santa Cruz), and Christopher Skinner (University of Manchester). Suzanne Hawley received a Hubble Fellowship, and former IGPP researcher Marco Tavani won a Gamma-Ray Observatory Fellowship for his work at IGPP. In addition to the IGPP postdoctoral fellows, Maurice Aufderheide, Stephane Charlot, and Ted Ressel, who are postdoctoral fellows in the Physics Department's E Division, work in the Astrophysics Research Center, participate in all Center activities, and contribute to the intellectual vitality of the group.

The Center hosts a large number of scientific visitors, many from the UC campuses and from around the United States and the world. These visits range from one day to one year. Some researchers who are affiliated with local institutions spend large, ongoing portions of their time in the Center. For example, Robert Becker (UC Davis) spends two to three days a week at the Center and contributes significantly to the scientific program.

The Center and its offices are housed in Building 319, which is close to the offices of many LLNL astrophysicists and is subject to minimal access controls. These features make the Center ideal for the many collaborations that have developed between UC researchers and LLNL scientists.

The Astrophysics Research Center has access to a variety of machines for computing. Most day-to-day work, which includes code development, image processing, and symbolic manipulation, is carried out on the Center's network of Sun workstations. This network comprises three server machines, twelve SPARCstations, and a few low-end workstations. One of the servers is on loan from UC Davis and is primarily used by Robert Becker to process radio astronomy data. We use this network for large-scale processing by exploiting the codes that use a large fraction of the network for parallel processing; such processing is especially effective at night, when most of the network is otherwise quiet and when the codes will not adversely affect the image processing work. In addition, much greater computing power is

available in other parts of LLNL: the Physics Department has an eight-processor Solbourne and a network of 14 IBM Risc stations, and Cray supercomputers are available in the Open Computing Facility and in the National Energy Research Supercomputer Center.

Research Highlights

The Astrophysics Research Center has developed a research program that exploits LLNL's traditional strengths in astrophysics and that opens up new areas not previously represented at the Laboratory. This research ranges from small-scale theoretical and observational projects carried out by the staff and postdoctoral fellows to large, collaborative ventures that involve scientists outside IGPP.

Laser Guide Stars

Claire Max, Clifford Choccol, and Herbert Friedman are working with four other LLNL collaborators and five collaborators from three UC campuses to develop laser guide stars for astronomical adaptive optics. The purpose of the project is to improve the angular resolution achieved at ground-based observatories by factors of 10 to 100.

The angular resolution of all ground-based telescopes with apertures larger than 10 to 20 cm is limited to about 1 s of arc because of turbulence in the atmosphere. In principle, one can use adaptive optics to correct for the wavefront distortions, which are measured with a wavefront sensor, by deforming a flexible secondary mirror to make the wavefront nearly flat. Then ground-based telescopes could be operated at or near their diffraction limits. For example, at a wavelength of 0.5 μm , the diffraction-limited resolution would be 0.04 arcsec for a 3-m telescope such as that at UC's Lick Observatory and 0.01 arcsec for a 10-m telescope such as the new Keck telescope. These represent improvements in resolution of factors of 25 and 100, respectively, relative to the atmospheric resolution of about 1 arcsec.

To accomplish this correction in the visible range, however, one needs a bright reference object within a few arcseconds of the object being imaged. The number of bright stars is such that, at most, only a few percent of the sky is accessible for diffraction-limited viewing, if nearby bright stars are used as the wavefront reference.

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

In the first phase of this long-term project, we used the copper-vapor-pumped dye laser, which was developed for LLNL's Atomic Vapor Laser Isotope Separation Program, to create an artificial star by illuminating the atmospheric sodium layer at 90 km. The guide star is fifth magnitude when the laser power is 1100 W and will be brighter once an optical pulse stretcher is in operation. The guide-star brightness has been measured as a function of laser power and central frequency, and preliminary wavefront sensor measurements have been performed using a wavefront sensor with 8-cm subapertures on a half-meter telescope.

Simultaneously, LLNL's Laser Isotope Separation Program is developing a high-repetition-rate laser that is compact in footprint and can be easily transported to a remote site, where it can be reassembled and perform reliably and reasonably efficiently. Once feasibility has been demonstrated on a 1-m telescope, this laser will be ready to field on a 3- to 4-m system at a site such as UC's Lick Observatory. The long-term goal is to establish a laser guide star system on the Keck telescope, operated by UC and the California Institute of Technology at Mauna Kea, Hawaii.

The MACHO Project

The Massive Compact Halo Object (MACHO) project is an experimental search for the dark matter that makes up at least 90% of the mass of our galaxy. It was initiated at LLNL and now involves scientists from five institutions: Charles Alcock, Robyn Allsman, Timothy Axelrod, David Bennett, Kem Cook, and Hye-Sook Park at LLNL; Stuart Marshall and Christopher Stubbs of the Center for Particle Astrophysics at UC Santa Barbara; Kim Griest of the Center for Particle Astrophysics at UC San Diego; Saul Perlmutter and Will Sutherland of the Center for Particle Astrophysics at UC Berkeley; and Kenneth Freeman, Bruce Peterson, Peter Quinn, and Alex Rodgers of the Mount Stromlo and Siding Spring Observatories in Australia.

The dark matter that exists in our galaxy is distributed in a large, spherical halo. This matter emits no detectable radiation, so its constitution is unknown. Most hypotheses for the constitution of dark matter involve speculations drawn from particle physics. Our experiment will search for planets, brown dwarfs, black holes, or any other massive object (collectively called MACHOs) in the mass range of $10^{-7} M_{\odot} < M < 100 M_{\odot}$. These objects represent the conservative hypothesis for the constitution of the dark matter.

If the dark matter is made of MACHOs, they will occasionally amplify the light from extragalactic stars by the gravitational lens effect. The amplification can be large (up to factors of a few). An event can be recognized by fitting a theoretical light curve to the observations (a three-parameter fit) and by the lack of color variation in the event (it is achromatic). Unambiguous recognition by microlensing thus requires at least 10 data points on the light curve and measurements in at least two filter bands. However, the expected event rate is low: Millions of stars must be monitored for several years to detect tens of events. The design goal is to detect at least 10 good events (maxima >0.25 magnitudes, >10 points/light curve, good three-parameter fit, no color variation) per year of operation, if MACHOs make up the halo. The experiment will operate for at least four years.

The MACHO project is operating with the 130-cm reflecting telescope of the Mount Stromlo Observatory near Canberra, Australia. Operating at prime focus with an innovative optical system gives a field of view 1 deg in diameter. By using a dichroic filter, we can image in two spectral bands simultaneously, thus doubling the effective exposure rate. The beams leaving the beam splitter are imaged onto mosaics of four 2048×2048 -pixel charge-coupled devices (CCDs) ($15 \mu = 0.6$ -arcsec pixels). The typical exposure is 300 s, followed by about 60 s to read out the CCD chips. The data rate from this experiment is large, averaging 4 Gbytes/night. The data are processed at the telescope using a dedicated computer system and software developed for the project. This system can measure the brightness of several million stars, twice per night, in the Large Magellanic Cloud. Working in the crowded regions at the central bar in the Large Magellanic Cloud, we can record more than 500,000 stars in one image.

Preliminary data analysis has shown that the system behaves well and, in particular, can recover all of the known periodic variable stars in the regions observed. Furthermore, there does not appear to be any unanticipated sources of background noise that will interfere with the search for MACHO events.

With this system, we expect to determine definitively whether the dark matter in our galaxy is made up of objects with mass in the range of $10^{-7} M_{\odot} < M < 100 M_{\odot}$.

Active Galaxies at High Redshift

Studies of active galaxies and their nuclei at high redshift encompass a variety of high-energy astrophysics disciplines, ranging from cosmology to galaxy formation and the origin and effects of galaxy activity.

Active galaxies at high redshift are most easily found through their association with extragalactic radio sources. In particular, previous work by Willem van Breugel, P. McCarthy (Observatories of the Carnegie Institute of Washington), K. Chambers (University of Hawaii), and G. Miley (Leiden Observatory) showed that radio galaxies at high redshift can efficiently be found by selecting radio sources that have steep spectra and that are relatively small (~ 20 arcsec). Systematic studies of such objects have resulted in two major discoveries.

The first discovery was that high-redshift ($z > 1$) radio galaxies often have unusually elongated, multimodal, blue optical continuum structures, which are nearly always aligned with their associated double radio sources. This discovery suggests that, at least in early cosmological epochs, radio galaxy activity is closely related to the parent galaxy morphology. In general, the optical continuum emission associated with a radio source may be the result of induced star formation, synchrotron emission, scattering of light from an active nucleus, inverse Compton scattering of microwave background photons by relativistic electrons, or thermal bremsstrahlung from shock-heated gas. In nearly all cases, the optical continuum is expected to be blue when compared to the spectrum of a normal elliptical galaxy. In addition, in the cases of synchrotron emission and scattering, one expects the continuum to be polarized. Although distant galaxies are difficult to study because they are optically faint, observations of several relatively nearby radio galaxies have now shown that both jet-induced star formation and scattering of light from active galactic nuclei (AGN) can indeed occur.

The second discovery was that radio galaxies already exist at very high redshifts. The current record holder is 4C 41.17, with $z = 3.80$. The spectral energy distributions of 4C 41.17 and similar high-redshift radio galaxies often show what is called a red bump at (rest) wavelengths > 300 nm, and a relatively flat spectral shape at shorter wavelengths. If the bulk of the red bumps are due to starlight, then according to stellar evolution models, the formation redshifts of the radio galaxies would be 4 to 5, which is marginally consistent with currently popular cosmologies.

Thus, radio galaxies are now known over a very large redshift range, and despite the close relationships between their optical and radio properties, they are still a good class of objects for galaxy formation and cosmology studies. However, a good understanding of the relationship between the optical and radio source properties is of key importance. To investigate these relationships further, we obtained a deep (three-hour) Hubble Space Telescope (HST) observation of the most distant galaxy.

Despite the flawed optics of the HST, we obtained a good image, the resolution of which was enhanced to 0.1 arcsec by using special image deconvolution techniques (Figure 1). The image showed that the bright optical emission at the center of the galaxy consists of several components. A radio image obtained at the

Very Large Array shows that the radio source also has three bright components (B1, B2, and B3), which closely correspond to the optical components seen with the HST. These observations considerably strengthened the apparent connection between the optical and radio properties of high-redshift galaxies and, thus, may further weaken their usefulness as probes for galaxy formation studies. Instead, they may be of great interest for exploring the origin of galaxy activity itself, in particular within the context of unified models of AGN and their possible connection to the one other class of enigmatic high-redshift AGN, quasars.

For example, in unified AGN models, the extended optical continuum observed in 4C 41.17 and other high-redshift galaxies would be due to scattered light from obscured quasar-type AGN into the line of sight above and below a thick obscuring disk or torus. Further HST and ground-based observations, including imaging and spectropolarimetry and 0.1-arcsec resolution multiband photometry, will be needed to investigate this.

Theoretical modeling of processes in AGN is another important aspect of our research program. Robert Rogers and G. Field (Harvard University) have explored the possibility that AGN accretion disks are dominated by loops of magnetic field. This model is motivated by x-ray observations of individual AGN, which reveal a highly variable, power-law continuum, and by the spectrum of the cosmic x-ray background, which may indicate the presence of cold gas near the x-ray-emitting region.

The magnetic field provides the viscosity necessary for material to accrete onto the central black hole and power the AGN. Above the accretion disk, a magnetic corona forms, and reconnection in the corona accelerates electrons to relativistic energies. This corona is a site for synchrotron emission and for the production of an x-ray power-law spectrum because of inverse Compton scattering of soft photons from the accretion disk. Some of these x rays are inverse Compton scattered again to produce gamma rays.

Figure 2 shows the resulting infrared to gamma-ray spectrum, which is qualitatively consistent with observations of individual AGN. The derived spectrum can be used to calculate the contribution of AGN to the cosmic x-ray, gamma-ray, and ultraviolet backgrounds. We found that the spectra of the x-ray and gamma-ray backgrounds could be explained by a population of such objects at redshifts between $z = 1$ and 3. Using the model parameters of this fit, we then calculated the

Figure 1. A linear contour representation of the deconvolved HST image of the most distant galaxy, 4C 41.17, at a redshift $z = 3.80$ (Ref. 6). The positions of the radio components B₁, B₂, and B₃ are marked by crosses. Compact optical components are denoted by H₁, H₂, H₃, and H₄. Note that there is an uncertainty of a few tenths of an arcsecond between the radio and optical components.

expected ultraviolet (UV) background at $z \sim 1$ and found that the predicted UV background is sufficient to ionize the intergalactic medium and suppress the Gunn–Peterson effect, as required by observation. In addition, the actual UV flux is consistent with the value derived from the proximity effect in which quasars cause additional ionization in Lyman- α clouds.

Current work involves modeling the magnetic field structure of magnetic-dominated accretion disks. Our work with G. Field focuses on the vertical and radial structure of the disk and the dependence of the spectrum on accretion rate.

Infrared Astronomy

Christopher Skinner, George Hawkins, and Margaret Meixner (UC Berkeley) have developed a program of observing cool, evolved stars with the Berkeley–IGPP Laboratory for Experimental Astrophysics mid-infrared array camera. The camera was used successfully on the United Kingdom Infrared Telescope (UKIRT) for the first time in November 1991 and again in May and June 1992. Two red supergiants, α Orionis and μ Cephei, were resolved for the first time in the 10- μ m region. We are using the results to constrain models of the circumstellar envelopes of the stars and to address the problem of the mass-loss mechanism. Several protoplanetary nebulae were also resolved for the first time, and we are using them with mid-infrared spectra obtained earlier at UKIRT, to determine the distances and hence the luminosity and mass-loss rates for asymptotic giant branch stars. This is the most successful mid-infrared camera that is in routine operation at a telescope.

In collaboration with Michael J. Barlow and Kay Justtanont (University College, London) and A. G. G. M. Tielens (NASA–Ames), Christopher Skinner has worked on analyzing mid-infrared spectra from UKIRT of several protoplanetary nebulae. The anomalous abundances and unusual combinations of dust features observed in some of these objects are consistent with their progenitors having undergone envelope burning, with convective dredge-up subsequently altering the photospheric abundances. We are analyzing another group of protoplanetary nebulae with unusual, and so far unidentified, mid-infrared dust emission bands.

This collaboration also reported the first astronomical detection of the methanol ice bands at 8.9 and 9.7 μ m, in mid-infrared spectra of the high-mass protostar AFGL 2136 taken at the UKIRT. The methanol ice abundance in such sources has been a subject of some controversy because the values determined from measure-

Figure 2. The calculated infrared to gamma-ray spectrum of a point on an accretion disk, which is qualitatively consistent with observations of individual AGN. This spectrum can be used to calculate the contribution of AGN to the cosmic x-ray, gamma-ray, and ultraviolet backgrounds.

ments of the bands at 3.53 and 6.85 μm differ by an order of magnitude. Measurements of the mid-infrared bands were consistent with the 3.53- μm band, casting doubt on the identification of the 6.85- μm band, which was previously considered the best indicator of methanol ice in star-forming regions.

Searching for Asteroids

Charles Alcock, Kem Cook (Laboratory for Experimental Astrophysics at LLNL), Eugene Shoemaker (U.S. Geological Survey), and Ted Bowell (Lowell Observatory) are developing a new CCD camera to use for a preliminary search for near-Earth asteroids. For this project, we modified a camera that was developed for the MACHO project so it could be used in "scan" mode. In this mode, the camera and telescope system is moved rapidly along great circles across the sky, and the CCD chips are read out constantly. Scan mode is an effective way to cover very large regions of the sky with short exposures, which will be needed for our project. The camera will be installed on the 60-cm Schmidt telescope at Anderson Mesa, Arizona, and is expected to go into operation in about a year. The system is expected to greatly enhance the present discovery rate for near-Earth asteroids and will serve as a development stage for the much more ambitious Spaceguard project, which aims to detect more than 90% of all large ($>1\text{-km}$) near-Earth asteroids.

Center for Geosciences

The primary purpose of the IGPP–LLNL Center for Geosciences is to promote collaborative research in the earth sciences between LLNL and UC researchers. Many subdisciplines within the geosciences are used by LLNL's mission-oriented programs in national security and energy research. IGPP can draw on these capabilities and expertise and can act as a focal point for research in the more fundamental aspects of these areas. In doing so, we hope to consolidate the many talents and capabilities at LLNL and provide an easily identifiable avenue for LLNL–UC collaborations.

The Center for Geosciences is the physical and scientific focus for interactions with visitors from academic (UC and non-UC), industrial, and government geoscience research institutions. We continue to emphasize the physics and chemistry of the solid Earth, including seismology, geochemistry, experimental petrology, mineral physics, and hydrology, and we recently initiated an effort in geodesy.

Operational responsibilities for the Center are shared by George Zandt and Frederick (Rick) Ryerson. Zandt is a seismologist with interests in the Earth's upper-mantle and crustal structure, tectonics, and developing seismic underground imaging techniques. Zandt oversees research projects in seismology and observational geophysics. Ryerson is an experimental petrologist with interests in diffusion in rock-forming minerals, rheology of partially molten crustal rocks, and high-pressure and high-temperature mineral-melt phase equilibria. He oversees projects in geochemistry, mineral physics, and experimental geophysics.

In addition, John Rundle and Jim Berryman work in the Center. Rundle is interested in geodesy and in applying the modern physics of complex systems to problems in the earth sciences. Geodetic measurements are important in constraining crust and mantle dynamics, and their use in tracing glacial advance and retreat should also affect studies of global climate variations. Berryman is a physicist with interests in inverse theory and its application to geophysical problems. His research efforts include seismic and electrical impedance tomography and theoretical rock physics.

The Center for Geosciences is located in and partially supported by LLNL's Earth Sciences Department. It has strong ties with several programs in the Earth Sciences Department and in the Nuclear Chemistry Division, which is a major contributor of scientific expertise and facilities to support collaborative efforts in geochemistry. The Center is located in an area of the Laboratory that is subject to minimal access controls. This area houses the Center's library and several computer workstations for use by visitors and staff and is the focus of our activities in seismology and geodesy.

Research in geochemistry and experimental geophysics is conducted in facilities within the Earth Sciences Department and the Nuclear Chemistry Division. The newly opened Nuclear Chemistry facility houses an ion microprobe, an electron microprobe, an inductively coupled plasma–mass spectrometer, and clean laboratory facilities for preparing accelerator mass spectrometry samples. The laboratories for thermal ionization mass spectrometry also were reclassified to allow access by UC participants. The Earth Sciences' experimental facilities include the apparatus for high-pressure gas media deformation experiments, the piston cylinder and multi-anvil laboratories, and laboratories for measuring electrical conductivity and crystal growth, for diamond cell and cryogenic deformation experiments, and for x-ray diffraction analysis and infrared spectroscopy.

Three new postdoctoral researchers joined the Center for Geosciences in FY 1992. Annie Kersting (University of Michigan) is working with Rick Ryerson and Henry Shaw on the isotopic characteristics of island arc volcanoes. She took

part in field excursions to the Redoubt volcano in Alaska with John Eichelberger (University of Alaska) and sampled several Japanese island arc volcanoes with Richard Arculus (University of New England, Australia). She is performing radiogenic and stable isotopic analyses of these samples.

James Brennan (Rensselaer Polytechnic Institute) also joined the Center and is working with Henry Shaw, Rick Ryerson, and Douglas Phinney on a project to characterize the partitioning of trace elements between rock-forming minerals and fluids at high pressure and temperature. Charles Williams (University of Arizona) is working with John Rundle on modeling active deformation mechanisms in the Long Valley Caldera. Stanley Ruppert (Stanford University) is working with George Zandt on the structure and tectonics of the western United States.

During the summer of 1992, Bill Minarik (Rensselaer Polytechnic Institute) and Diana Fisler (Pennsylvania State University) visited LLNL as summer students. Minarik performed experiments to investigate the enhancement of effective bulk diffusion in mineral aggregates due to the presence of grain boundary fluids and melts. Some of his experiments were done in the multianvil press and were aimed at determining the textural relationships between potential core-forming melts and upper-mantle phase silicates. Fisler worked primarily with Mark Beeman on grain growth and deformation of quartzites. She also performed electrical conductivity experiments with Al Duba.

Daniel Farber (UC Santa Cruz) is continuing his experiments on cation diffusion in olivine at high pressure with his campus advisor Quentin Williams and Rick Ryerson. In addition, two new students from UC Santa Cruz, Craig Lundstrom and Clifford Gill, are investigating trace-element partitioning in mineral-silicate melt and mineral-carbonate melt in conjunction with Henry Shaw, James Brennan, and Rick Ryerson.

In the area of geophysics and tectonics, Charles Carrigan, a geophysicist in the Flow and Transport Group, has been working on a new model of magma transport with Gerald Schubert (UC Los Angeles). Carrigan also collaborated with George Zandt on upper-mantle convection instabilities (described later in this section). Chris Sanders (Arizona State University) and his student, Stephen Ponco, spent the summer here under the auspices of the Association of Western Universities. They worked with George Zandt on a seismic investigation of the crustal structure of Long Valley. Kevin Mayeda, a postdoctoral researcher from the University of Southern California, has joined the Seismic Verification Group to model coda-wave propagation. Another postdoctoral researcher in the Seismic Verification Group is William Walter, who is working with Charles Ammon (UC Santa Cruz) on developing regional waveform modeling techniques to determine earthquake source parameters and earth structure. John Rundle has continued his collaborations with William Klein (Boston University) on applying statistical mechanics to earthquakes and crack propagation. Also working with Rundle on inversion of geodetic data near faults is Hadley Johnson (Scripps Institute of Oceanography, UC San Diego). Mark Harrison and An Yin (both of UC Los Angeles), Peter Copeland (University of Houston), William Kidd (State University of New York, Albany), and Rick Ryerson took part in a field excursion to Tibet in September 1992. Herve Leloup (UC Los Angeles and University of Paris) also visited LLNL to work on various aspects of the pressure-temperature history of the Ailao Shan-Red River Shear Zone in China.

Kevin McKeegan (UC Los Angeles) and Douglas Phinney (Nuclear Chemistry, LLNL) are continuing to build a library of relative ion yield standards for quantitative analysis by secondary ion mass spectrometry. McKeegan is also working with Rick Ryerson on measuring diffusion in rock-forming minerals and melts.

Research Highlights

Tibetan Tectonics

Part of the convergence in the Indo-Asian collision has been accommodated by major intracontinental thrusts in the Himalaya Mountains, such as the Main Central and Main Boundary thrusts. However, the existence of a south-directed intracontinental thrust system in southern Tibet, the Gangdese thrust system, has been postulated on the basis of thermochronological results and geologic relationships, in particular the juxtaposition of Indian continental margin deposits (Tethyan) against the Andean-type plutonic belt (the Gangdese batholith). In September 1992, Mark Harrison and An Yin (both of UC Los Angeles), Peter Copeland (University of Houston), William Kidd (State University of New York, Albany), and Rick Ryerson (IGPP) went to Tibet to investigate several features that may be related to movement along the Gangdese thrust.

Field observations and paleo-unroofing studies indicate a clear negative correlation between the preservation of forearc sediments (Xigaze Group) and the magnitude of exhumation, indicating that maximum uplift is responsible for uplifting and eroding these sediments. West of Renbu (90°E, 29°N, Figure 3), the style of deformation in the hanging wall of the Gangdese thrust system is characterized by south-directed thrust faults and folds along the southern part of the Xigaze Group and by north-vergent thrusts and folds along its northern margin. East of Renbu, crustal shortening is concentrated along the north-dipping Gangdese thrust system. This shortening brings Gangdese plutonics directly over the Tethyan sedimentary rocks and thus eliminates exposure of the forearc sediments. Near Zedong (92°E, 29°N) in the easternmost observed part of the Gangdese thrust system, the fault zone is characterized by several hundred meters of mylonitized granite and sedimentary rocks. In contrast, the Gangdese thrust near Xigaze is characterized by cataclastic deformation.

Figure 3. Stratigraphic cross section west of Renbu (90°E, 29°N), showing the style of deformation in the hanging wall of the Gangdese thrust system. We found south-directed thrust faults and folds along the southern part of the Xigaze Group and north-vergent thrusts and folds along its northern margin. East of Renbu, crustal shortening is concentrated along the north-dipping Gangdese thrust system. This shortening brings Gangdese plutonics directly over the Tethyan sedimentary rocks and thus eliminates exposure of the forearc sediments. R = Renbu, Z = Zedong.

Excellent exposures of the Gangdese thrust east of Xedong contain abundant kinematic indicators, such as asymmetric folds, asymmetric boudinage, and minor south-directed thrusts. These features unambiguously demonstrate the south-directed nature of the thrust, which currently dips about 35 deg to the north. Directly below the mylonitic shear zone of the Gangdese thrust is a sequence of unmetamorphosed conglomerates (>1 km). The conglomerate cobbles are predominantly marble but also contain rare cobbles of Gangdese plutonics. This important structure has previously been unrecognized mainly because of the younger north-directed thrust system, the Renbu–Zedong thrust (RZT), that truncates the Gangdese thrust. The RZT obscures the trace of the Gangdese thrust and in at least one locale, juxtaposes Tethyan rocks over unconsolidated gravels.

On the basis of our existing thermochronological results, we infer that significant motion along the Gangdese thrust system occurred between 25 and 18 million years ago. The geologic relationships characterizing the rocks east of Zedong are also shared by those near Mount Kailas, about 1100 km to the west, where we have also documented early Miocene uplift. Our finding suggests that the Gangdese thrust system was active over at least 1100 km. Absence of the Xigaze Group implies a minimum displacement of about 20 km along the Gangdese thrust. This crustal thickening event explains the rapid unroofing of an equivalent section in the eastern Gangdese and thus precludes other mechanisms (e.g., climate change, tectonic denudation) as the primary cause of the early Miocene transition in cooling rate. The variation in the magnitude of displacement along the strike of the Gangdese thrust may result from the transfer of displacement to thrusts in the Tethyan Himalayas, the irregularity of the northern boundary of the Indian continent, or the mismatch of curvature of the Gangdese arc and the Indian continent.

Upper-Mantle Viscosity and Small-Scale Convection under California

The possible presence and influence of small-scale upper-mantle convection in oceanic and tectonically active continental regions are still a widely debated problem. Seismic tomography is providing some of the first direct evidence on global mantle convection patterns, but higher resolution images are required to investigate small-scale convection in the upper mantle. We combined tectonic and tomographic data associated with the central California upper mantle to obtain time- and length-scale constraints on the development of a localized, thermal boundary layer instability within the mantle. We used these constraints with an analytical model of boundary layer instability that is supported by more detailed numerical experiments, to predict a characteristic range of viscosity for the asthenosphere (the “weakest” mantle layer) under California (Figure 4). This range of 5×10^{18} to 5×10^{19} Pa · s implies that a low-viscosity layer exists under California and probably under most of western North America and other tectonically active continental regions. Although the tectonic situation associated with this particular thermal instability is rather unusual, the instability is likely to typify the onset of the small-scale regime of high Rayleigh number convection in the Earth’s asthenosphere.

Figure 4. Schematic cross section of the development of an unstable thermal boundary layer and the formation of a "blob" in the upper mantle beneath California. As the Gorda Plate moves northwestward with respect to North America, low-viscosity asthenosphere upwells into the slab window, the space previously occupied by the slab. The new mantle material cools conductively, which causes the density to increase. When this new layer of denser mantle reaches a critical thickness, it becomes convectively unstable and "drips" off into the underlying mantle.

References

1. Nellis, W. J., A. C. Mitchell, P. C. McCandless, D. J. Erskine, and S. T. Weir (1992), "Electronic Energy Gap of Molecular Hydrogen from Electrical Conductivity Measurements at High Shock Pressures," *Phys. Rev. Lett.* **68**, 2937.
2. Ross, M., F. H. Ree, and D. A. Young (1983), "The Equation of State of Molecular Hydrogen at Very High Density," *J. Chem. Phys.* **79**, 1487.
3. Gratz, A. J., L. D. DeLoach, T. M. Clough, and W. J. Nellis (1993), "Shock Amorphization of Cristobalite," *Science* **259**, 663.
4. Gratz, A. J., W. J. Nellis, J. M. Christie, W. Brocious, J. Swegle, and P. Cordier (1993), "Shock Metamorphism of Quartz with Initial Temperatures -170 to +1000°C," *Phys. Chem. Minerals* **19**, 267.
5. Gratz, A. J., W. J. Nellis, and N. A. Hinsey (1992), "Laboratory Simulation of Explosive Volcanic Loading and Implications for the Cause of the K/T Boundary," *Geophys. Res. Lett.* **19**, 1391.
6. Miley, G. K., K. C. Chambers, W. J. M. van Breugel, and F. Macchetto (1992), "Hubble Space Telescope Imaging of Distant Galaxies: 4C 41.17 at $z = 3.8$," *Astrophys. J. Lett.* **401**, L69.

Section III. Research Summaries of Collaborative Projects

High-Pressure Sciences

Deformation and Neutron Diffraction Texture Analysis of Ice

Principal Investigator: Hans-Rudolf Wenk (UC Berkeley)

LLNL Collaborators: William B. Durham, Andrew J. Gratz, and William J. Nellis

Other Collaborators: Stephen H. Kirby and Laura A. Stern (U.S. Geological Survey, Menlo Park, CA)

Student: Kristin Bennett (UC Berkeley)

We used neutron diffraction techniques to analyze the texture and identify the phases of experimentally deformed deuterated ice. We deformed ice I, ice II, and ice I mixed with hard particulates, using the high-pressure, low-temperature gas apparatus unique to LLNL's Experimental Geophysics Group. Then at the Manuel Lujan, Jr., Neutron Scattering Center at Los Alamos National Laboratory, we measured pure ice I deformed in three flow regimes divided by temperature, using time-of-flight pulsed neutrons at liquid nitrogen temperatures. We found that ice I shortened 30% at 180 K by quasi-static deformation does not develop a strong texture, but at 220 and 256 K, it develops preferred orientation.

Abstract

We also deformed deuterated ice I in LLNL's two-stage light-gas gun and used the pulsed neutron source at Los Alamos to identify the phases. We are continuing to study the micromechanics of ice so we can interpret the macroscopic ice flows on Earth and the geophysical deformations on icy bodies in the outer solar system. In the future, we will use monochromatic neutrons to measure samples of ice mixed with hard particulates and a sample of pure ice I at the National Institute of Standards and Technology.

Ice I deformed at high pressure and low temperature is characterized by three different flow regimes. We are studying the creep properties of ice I to help us interpret the flow of ice on the surface of the Earth and on the surfaces and the interiors of ice-rich moons. Optical images collected by the Voyager spacecraft mission in 1979 revealed deformation features on Ganymede and Callisto that are 50% by weight water ice. At present, the artificial satellite Galileo is on a mission to examine the surfaces of these bodies more closely. We are investigating the creep laws of ice in much greater detail with texture analysis.

Objectives

Texture, or preferred crystallographic orientation, contributes to our understanding of the micromechanical physics of deformation and recrystallization. In FY 1991, we completed pilot measurements of an ice I and an ice II sample. For FY 1992, our first goal was to complete a suite of measurements of ice I using an improved experimental approach at Los Alamos. Our second goal was to examine the materials and conditions that more directly apply to icy bodies, such as ice mixed with hard particulates and ice deformed by shock loading.

Progress

We characterized the anisotropy in deformed ice by neutron diffraction, which is essential to quantify ice-flow laws. Low-porosity, polycrystalline samples with a controlled grain size were molded at the U.S. Geological Survey. To avoid incoherent scattering when placing a deformed sample in the neutron beam, we substituted deuterium for hydrogen in all samples. We deformed pure deuterated ice I in three flow regimes. Three samples were shortened by 30% at a strain rate of $3.5 \times 10^{-4} \text{ s}^{-1}$ with a confining pressure of 50 MPa (0.5 kbar) and temperatures of 180, 220, and 256 K. We deformed another pure ice I sample at the same strain rate and confining pressure and a temperature of 220 K but with half the starting grain size. Three more ice I samples mixed with hard particulates were shortened by approximately 25% at a strain rate of $3.5 \times 10^{-4} \text{ s}^{-1}$ with a confining pressure of 50 MPa and a temperature of 220 K. In addition, we transformed ice I to ice II and shortened the sample by approximately 35% at a rate of $3.5 \times 10^{-4} \text{ s}^{-1}$ with a confining pressure of 190 MPa and a temperature of 195 K. We also shock-loaded five deuterated, pure ice I samples at peak pressures of 0.6, 1.2, 1.5, 2.4, and 5 GPa at temperatures of approximately 100 K.

Using neutron diffraction, we characterized three ice samples at about 77 K. We prefer to use neutron diffraction, rather than x-ray diffraction, because neutrons can penetrate the 2.5-cm-long samples with low absorption. Samples were mounted with the axis of compression in a plane parallel to the incident neutron beam and were rotated perpendicular to it by a motor controller. To record the texture, we measured scattering as a function of orientation and used about 10 orientations for each sample. To improve the statistics, we scanned ± 5 deg for each orientation and averaged the intensity.

Because of electronic inefficiencies in the high-angle detectors at Los Alamos, only qualitative texture analysis is possible for d-spacings between 0.3 and 0.4 nm. Using two backscattering detector banks, we made measurements for (110), (004), (104), and (211) poles or directions. Figure 1 shows diffraction intensity vs orientation angle, in the form of the (004) vs (110) ice poles relative to the (006) pole of our internal standard, for the three pure ice I samples deformed to 30% strain at different temperatures. Figure 1 demonstrates the stronger fabric development in ice deformed at higher temperatures compared with that deformed at low temperature (180 K).

To identify the phases, we measured four of the five shock-loaded samples by neutron diffraction. Samples were mounted with the axis of the shock front perpendicular to the incident neutron beam, so that the entire sample was immersed in the beam. The time-of-flight pulsed neutron source allowed us to collect a complete powder pattern instantaneously. Preliminary results suggest that all shocked samples were crystalline.

Figure 1. Axial distribution function of (004) ice vs (110) ice vs (006) standard poles. This figure demonstrates the stronger fabric development in ice deformed at higher temperatures compared with that deformed at low temperature (180 K).

Additional neutron diffraction measurements will be performed at the National Institute of Standards and Technology (NIST). Because the beam is monochromatic, we need three to four pole measurements to calculate the orientation distribution function and the texture of the other diffraction peaks. We will measure one pure ice sample that was previously measured at Los Alamos and compare the results with those using the NIST technique.¹

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1. Wenk, H.-R., and G. R. Canova (1991), "Texture Evolution in Minerals: Modeling and Experimental Results," in *Modeling the Deformation of Crystalline Solids*, T. C. Lowe, A. D. Rollett, P. S. Follansbee, and G. S. Daehn, Eds. (TMS-AIME, Warrendale, PA), p. 349.

References

Preparation and Characterization of Iron Films on Sapphire and Diamond

Principal Investigator: David J. Webb (UC Davis)

LLNL Collaborators: Choong-Shik Yoo and Neil C. Holmes

Student: Christopher Pike (UC Davis)

Abstract

As part of a project to measure the melting temperature of iron at pressures relevant to the Earth's core, we are studying the physical characteristics of thin films of iron to be used for shock-temperature measurements. Shock temperature is obtained by measuring the spectral dependence of light emitted from the shocked iron film. In our study, the film density was excellent, being within about 1% of the value for bulk iron. The interface between the iron film and the diamond substrate was sharp, less than 5 nm in width. We chose a diamond substrate to retain optical transparency at high shock pressures. The electrical resistivity and scanning electron microscope studies indicated that the iron film grows smoothly and uniformly on diamond but in a granular fashion on sapphire. This result suggests that diamond is the better substrate. Initial measurements at LLNL of the temperatures produced in shock studies of these films suggest that, indeed, diamond is an excellent substrate.

Objectives

The melting temperature of pure iron at the pressures in the Earth's core is an upper limit on the temperature at the boundary of the Earth's inner and outer cores. To better understand the energy balance and the resulting dynamics of the Earth, we need a good estimate of the temperature of liquid iron at high pressures. However, estimates of this melting point by various researchers differ by thousands of degrees. The goal of our study is to grow thin iron films on transparent substrates of diamond or sapphire and use them in shock-wave studies to measure the melting temperature of iron at high pressures. To understand the shock-wave data obtained by this method, we must know the film density quite well, and the film-substrate interface must be somewhat thinner than the optical penetration depth of iron, about 5 nm. Thus, we wanted to measure the film density to within 1% and characterize the interface in terms of composition, microstructure, and size.

Progress

To date, we have studied the properties of iron films deposited on sapphire and diamond substrates. The densities of the films were within about 1% of that of bulk iron, and x-ray diffraction showed that our iron crystals had lattice constants within 0.1% of that of pure iron. However, we have evidence that the properties of the interface between the iron film and its substrate are better for diamond substrates than for sapphire substrates.

Iron films deposited on sapphire substrates held at room temperature did not adhere well to the sapphire. Heating the substrates helped the adhesion, but the iron formed disconnected islands when it was deposited on high-temperature sapphire. For instance, a 20-nm-thick iron film deposited at 450°C on sapphire was insulating, which indicated the absence of an electrical connection between one edge of the film and the opposite edge. The film becomes electrically connected through the agglomeration of these islands when the film thickness is increased to about 40 nm.

However, voids may still exist near the iron–sapphire interface, so the density of the first few tens of nanometers may be somewhat less than that of the bulk film. This situation is undesirable.

The films grown on diamond are appropriate for shock-temperature measurements. We deposited films on diamond substrates heated to 350°C and measured the interface with Auger sputter profiling. In this experiment, we determined the composition of the surface, the top 1 to 2 nm of the film, by measuring the composition profile as a function of depth. The data show that the interface is at most 5 to 6 nm thick. There are two possible explanations for this result: (1) If the substrate is rough on this scale, the diffusion of iron into the diamond may occur over a much thinner distance than 5 to 6 nm; or (2) the interface may represent an actual composition gradient across a diffused interface. In either case, the interface should not cause a problem with the shock-temperature measurements.

Initial shock studies of these films on diamond substrates have been carried out at LLNL. The shock temperature increases as the shock reaches the iron–diamond interface and remains constant until the shock reaches the other face of the diamond substrate.

Realistic Theoretical Simulation of Temperature–Pressure Quenching

Principal Investigator: Ching-Yao Fong (UC Davis)

LLNL Collaborator: Christian Mailhot

Student: In-Chu Chang (UC Davis)

Abstract

We want to develop theoretical computations to predict the realistic quenching of high-temperature–high-pressure phases in high-pressure experiments. If high-pressure phases can be retained at ambient pressure by quenching (rapidly releasing the temperature and pressure), then we may be able to fabricate materials with potentially novel properties. Thus, we calculated the equations of state (energy vs atomic volume) using first-principles total-energy methods. Two attractive materials are BeH_2 and nitrogen. We calculated two phases of BeH_2 : the observed phase at ambient pressure and the Laves-type phase. We also calculated the cubic polymeric phase of solid nitrogen. Then we fitted the total-energy calculations for nitrogen to the parameters of the Stillinger–Weber potential and tested the calculations against measured vibrational spectra of solid nitrogen at high pressures.

Objectives

We want to develop an efficient theoretical method to predict the formation of high-pressure phases that might be retained by quenching from high temperatures and high pressures.¹ Thus, our first objective was to verify that our computer programs using first-principles total-energy calculations predict, at normal conditions, the observed phase with the lowest energy state. In addition, higher energies should be calculated for the other possible crystal structures or metastable states. Our second objective was to test the programs for economically and effectively generating initial high-pressure phases before the quenching process begins. An important issue here is obtaining and evaluating an effective phenomenological potential for the interatomic interaction energy.

Progress

We carried out first-principles total-energy calculations of the observed and the Laves-type phases of BeH_2 at ambient pressures and of the cubic polymeric phase of solid nitrogen at high pressures. By comparing our earlier results for BeH_2 with our calculations for the calcium–carbide and fluorite-type phases, we confirmed that our first-principles total-energy calculations successfully predict the observed phase of BeH_2 , that is, the phase having the minimum total energy at ambient conditions. This accomplishment is significant because of the complexity of the BeH_2 structure.

For solid nitrogen, we calculated the polymeric phase with a body-centered cubic structure or unit cell. We determined two sets of parameters for the Stillinger–Weber potential by fitting the calculated total energies vs unit-cell volume for both the polymeric and the previously calculated black-phosphorous (black-P) phases. Interactions between the nearest and the second-nearest atomic neighbors are taken into account by treating the strengths of the short-range and long-range components of the interaction potential as a function of the interatomic distance. Figure 1 shows our results for the potential of the black-P phase vs lattice constraint. The minimum in this curve corresponds to the expected lattice parameter.

Then using the lattice dynamic program that we developed in FY 1991, we calculated the vibrational spectra of the two nitrogen phases at $q = 0$, where q is the phonon momentum. We also calculated the highest vibrational frequency of a nitrogen molecule in these solids for the respective phases and compared the results to the measured vibrational frequency of a nitrogen molecule. Table 1 summarizes the results of the calculated frequencies of the two phases of solid nitrogen and compares them to some experimental data.²

Figure 1. The fitted total energy using the Stillinger–Weber potential compared to the first-principles total-energy results for the black-P phase of solid nitrogen. The minimum corresponds to the expected lattice parameter at zero pressure. Higher pressures correspond to lattice parameters below the minimum.

Table 1. Comparison of calculated frequencies of two phases of solid nitrogen, a nitrogen molecule, and experimental data.

	Bond length (nm)	Pressure (GPa)	Nearest neighbor frequency (cm ⁻¹)	Frequency (cm ⁻¹)
Cubic polymer phase	0.13931	144.7	1564.72	1635.2
Black-P phase	0.15293	107.4	1119.77	1584.93
Nitrogen molecule	0.10975	—	2328.0	—
Experimental data ^a	—	126.1	2382.5	—

^aExtrapolated Raman spectra of solid nitrogen.

The larger the bond length, the smaller the frequency. Thus, the 33 and 50% discrepancies of the cubic polymeric and black-P phases compared to the known molecular frequency occur because the calculated bond lengths are different than expected. We extrapolated the calculated experimental results from the Raman measurements at the average theoretical pressure because the data did not cover the pressure range in the theory. The theoretical values are about 30% smaller, which can be considered reasonable because of the extrapolation.

In conclusion, we confirmed that our programs can correctly predict the lowest total-energy phase and calculate the metastable phases. The phenomenological interatomic potentials obtained by fitting the total-energy results provide reasonable predictions of vibrational frequencies of the different phases. The potentials can be used to determine initial configurations for the time-consuming first-principles total-energy calculations in simulating the high-pressure experiments.

References

1. Gallup, R. F., C. Y. Fong, A. K. McMahan, and C. Mailhot (1991), "Electronic, Structural, and Mechanical Properties of Possible Metastable Phases of Beryllium Hydride," *High Pressure Res.* **6**, 291.
2. Mailhot, C., L. H. Yang, and A. K. McMahan (1992), "Polymeric Nitrogen," *Phys. Rev. B* **46**.

The Computational Modeling of the Shock Compaction of Ceramics

Principal Investigator: David J. Benson (UC San Diego)

LLNL Collaborators: Robert Tipton and William J. Nellis

We used an arbitrary Lagrangian Eulerian computer program developed at LLNL to investigate the shock compaction of ceramic powders in shock-compression experiments. The morphology of the powders in the experiments ranged from nearly spherical to irregularly shaped particles. We wanted to model discrete individual particles so we could study their interactions in detail. Therefore, we developed a computer program to generate a random size and spatial distribution of cylindrical and rectangular particles representative of those used in the experiments.

Abstract

The shock synthesis and compaction of advanced materials from powders is an area of intense research. Shock loading can be obtained using gas guns and explosives. Little numerical simulation has been performed on the micromechanical scale to characterize what happens to powders during shock compression. Our goal is to understand the shock-induced micromechanics of powders well enough so that we can design the shock process to maximize the material yield and thus improve the structure and properties of shock-compressed materials through computational design.

Objectives

We investigated the dynamic compaction of powders, using Eulerian hydrocodes to simulate the shock compaction of a few hundred discretely modeled particles by a copper plate traveling at 1.0 km/s. We modeled the particles as cylinders in two dimensions so we could analyze the interaction of a relatively large number of particles.

Progress

The shape of the particles is a function of the method used to synthesize them. For example, spherical powders are often available commercially; we modeled them as circular disks. Rapidly solidified powders have particles with irregular shapes; we modeled them as rectangles. We obtained the particle-size distribution data from powders that were compacted by Joanna McKittrick and William Nellis in another IGPP project.

To simulate the process of loading the powder into a capsule for gas-gun experiments, we developed an algorithm to calculate the initial size and spatial distribution of the powder particles. The experimental procedure is to pour the powder into a capsule and then tap the capsule to settle the powder particles to a repeatable and representative density. Our algorithm pours and “taps” the powder into the capsule one particle at a time, where the numerical capsule is the region in space that fills with particles. The pouring algorithm is very general and can handle arbitrary, simply connected polygons.

Figure 1 shows the calculated initial and final states for a copper powder. This calculation was performed with RAVEN, a Eulerian code developed by David Benson, and agrees qualitatively with the behavior observed in experiments. The upper boundary, which moves downward at a velocity of -1.0 km/s, acts as a rigid copper impact plate. Although all the particles are made of copper, each

particle is assigned a material number that is different from the material numbers of particles surrounding it so that the boundaries of particles can be tracked during the calculation.

As shown in Figure 1b, the voids are filled by jets of material from the particles immediately above the voids. The lengths of the jets appear to be proportional to the diameter of the voids. This observation provides a micromechanical explanation of a classical result from continuum physics that lower density powders are heated more during dynamic compaction than higher density powders. Large voids imply large jets and a correspondingly high amount of heating from the plastic deformation of particles. The jets also form vortices in several locations, a phenomena that has been observed in explosive welding experiments.

Figure 1. (a) Initial size distribution of copper particles. Initial porosity is about 25%; particle sizes range from 0.4 to 25 μm . (b) The same particle distribution as in (a) but compressed by a rigid copper plate 0.1 μs after the plate is incident from above at -1 km/s . This compressive velocity corresponds to a pressure in the copper powder of about 30 GPa (300 kbar) and an impact pressure of about 40 GPa. The computational method is readily adapted to a wide range of compressive velocities and material structures.

We are performing calculations for ceramic powders with CALE, a Eulerian hydrocode developed by Robert Tipton at LLNL, and using a material model and data supplied by Daniel Steinberg of LLNL. We are using the same particle distributions for all of the materials so that we can evaluate the roles of the particle spatial distribution, particle morphology, and material properties on the shock-compaction process. We believe these computational simulations will improve our ability to understand the structures of the compacted materials.

Shock Compaction of Nanocrystalline and Glassy Oxide Ceramics

Principal Investigator: Joanna McKittrick (UC San Diego)

LLNL Collaborator: William J. Nellis

Student: Bahadır Tunaboylu (UC San Diego)

Abstract

The shock compaction of Al_2O_3 - ZrO_2 binary and ternary compositions resulted in dense, crack-free or nearly crack-free samples for pressures of ≤ 12.6 GPa. We believe that plastic deformation of α - Al_2O_3 by dislocation slip accommodated most of the tensile stresses created during release shock waves, thereby filling the available voids in the powder. We found a metastable, high-pressure phase of ZrO_2 , which was formed from the monoclinic polymorph at and above shock pressure of 6.3 GPa. Higher pressures extended the transformation but also disrupted the samples. The compaction of glassy and nanocrystalline starting materials showed good structural integrity, although the bulk density was relatively low. Microstructural analysis showed that the fine and uniform microstructures are retained after the compaction for all compositions.

Objectives

Shock compaction is an alternative and promising technique for fabricating dense ceramic bodies with fine grain sizes and uniform microstructures. In shock compaction of refractory powders, densification is thought to be achieved by plastic deformation of Al_2O_3 particles, which occurs at relatively low temperatures. Grain growth is essentially nonexistent, in contrast to conventional sintering (densification) techniques, which involve heating to high temperatures. Shock compaction produces heterogeneous surface heating, thermal quenching, and bonding between ceramic particles, while maintaining the interior of the particles at relatively low temperatures. These phenomena give shock compaction the potential to synthesize bulk materials with unique microstructures and metastable phases, which cannot be obtained with traditional processing.

The purpose of this study was to investigate whether Al_2O_3 - ZrO_2 ceramics could be fabricated through shock compaction and to determine the effectiveness of this technique in obtaining uniform microstructures in dense, crack-free samples. We selected the eutectic composition in the Al_2O_3 - ZrO_2 system as a prototype because both commercial and rapidly solidified powders are available. When we rapidly solidified Al_2O_3 - ZrO_2 compositions, metastable amorphous, nanocrystalline, or submicrocrystalline ZrO_2 phases formed in the as-quenched condition. Shock compaction should be a viable technique to retain the nanostructures in bulk compacts. The fine-grained microstructures are expected to produce interesting physical properties. We extended the treatment to examine two additional ternary eutectics in the Al_2O_3 - Y_2O_3 - ZrO_2 and the Al_2O_3 - SiO_2 - ZrO_2 systems.

Progress

Shock pressures below 19.3 GPa (193 kbar) yield dense, crack-free or partially cracked samples. Figure 1 shows an optical micrograph of a dense, crack-free Al_2O_3 - ZrO_2 sample compressed at 6.3 GPa (Ref. 1). At increasingly higher pressures, macrocracking progresses to full powder formation. A critical transformation

range occurs between 20 and 30 GPa, above which only powders are formed, independent of the composition of the powder. Optical micrographs reveal that the macrostructures of consolidated powder specimens contain no noticeable macro-cracking major flaws in these samples. Our study demonstrates that $\text{Al}_2\text{O}_3\text{-ZrO}_2$ ceramics can be fabricated by shock compaction to relatively high densities with good interparticle bonding.

In examinations using transmission electron microscopy, we found that the ZrO_2 agglomerates were compacted into dense, large particles and the $\alpha\text{-Al}_2\text{O}_3$ grains were extensively distorted. The generation of dislocations in $\alpha\text{-Al}_2\text{O}_3$ grains appeared to aid the plastic deformation of this material and avoided fracture at lower pressures. Since the ZrO_2 is harder than Al_2O_3 and not fractured, our relatively high densities were probably achieved by plastic deformation of Al_2O_3 grains flowing around ZrO_2 particles and thereby filling interparticle voids during the passage of shock waves. We also observed highly deformed Al_2O_3 grains in examinations using scanning electron microscopy.

The fragmentation is prevalent above pressures greater than 12 GPa for the conventional $\text{Al}_2\text{O}_3\text{-ZrO}_2$ powders used in this study. However, a shock pressure of 12.4 GPa led to a coherent compact with the relatively low densities ($\rho_{\text{th}} \approx 55\%$) of rapidly solidified powders. In Figure 1, the porous nature of the bulk is readily observed, and the grains do not show any distortion, which indicates a lack of plastic deformation. Because of the relatively low density of this compact, the consolidation mechanism is yet to be determined. Each grain consists of light and dark areas, which are the ZrO_2 and Al_2O_3 regions, respectively.

Figure 1. Optical micrograph of commercial $\text{Al}_2\text{O}_3\text{-ZrO}_2$ powder compacted under 6.3-GPa shock pressure. The sample is crack-free and has a theoretical density of about 88%.

X-ray diffraction analyses of starting powders and the shocked materials showed that monoclinic ZrO_2 underwent a shock-induced phase change. The phase transformation started at shock pressures of about 6.3 GPa, and its extent increased as shock pressures increased. We have proposed a revised pressure–temperature phase diagram for the ZrO_2 system on the basis of a literature survey and what we have observed.

References

1. McKittrick, J., B. Tunaboylu, J. D. Katz, and W. J. Nellis (1992), “ Al_2O_3 – ZrO_2 Ceramics with Submicron Microstructures Obtained through Microwave Sintering, Plasma Sintering, and Shock Compaction,” *Mat. Res. Soc. Symp. Proc.* **274**, 149.

Dynamic High-Pressure Compaction of High-Temperature Superconductors

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

LLNL Collaborator: William J. Nellis

Students: Christopher L. Seaman, Lisa M. Pau'ius, and Seungho Han (UC San Diego)

Abstract

We have continued our research on the effects of shock compaction on high-temperature superconductors with the ultimate goal of producing specimens with high transport critical current densities. Because shock compaction can be used to introduce defects into these materials in a controlled manner, samples that have been shock-compacted can be used to study the fundamental nature of flux pinning in high-temperature superconductors. With this goal, we grew high-quality single crystals of Pr-doped $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ that had been characterized prior to shock-compaction. To minimize the breakage that occurred during previous compactions, we studied several techniques for loading the crystals. We are preparing these crystals for shock compaction and will characterize them to determine the effects of compaction on the flux-pinning energy and the critical current density.

Objectives

The greatest obstacle preventing the widespread use of materials with a high superconducting critical temperature (high- T_c) is their relatively low critical current densities, J_c . Our previous studies have demonstrated the potential of shock compaction as an important technique in producing bulk ceramic superconductors with high J_c (Ref. 1). In addition, numerous studies have shown that chemical doping also increases flux-pinning energies, U , and thus J_c . In particular, recent work has shown that low concentrations of praseodymium doping ($x \leq 0.2$) increase the pinning energy at a rate dU/dx of about 1 eV/Pr in the $\text{Y}_{1-x}\text{Pr}_x\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$ system. The compound $\text{Y}_{1-x}\text{Pr}_x\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$ is of considerable interest because the substitution of praseodymium for yttrium suppresses T_c and increases J_c . Understanding the mechanisms of this suppression should yield valuable insight into the mechanism of high-temperature superconductivity itself.

Our objective is to investigate the combined effects of chemical doping and structural defects caused by shock compaction on the critical current density and the flux-pinning energy of the $\text{Y}_{1-x}\text{Pr}_x\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$ system. In this study, we addressed the following issues:

1. What is the fundamental nature of flux pinning in the high- T_c superconductors?
2. Do the increases in pinning energy from chemical doping and structural defects add when combined?
3. What is the mechanism of T_c suppression in $\text{Y}_{1-x}\text{Pr}_x\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$?

Progress

We have developed a new technique for growing the desired superconducting single crystals in zirconia trays. First, we prepare polycrystalline powders of $\text{Y}_{1-x}\text{Pr}_x\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$ and mix them with BaCO_3 and CuO to give a ratio of $(\text{Y}_{1-x}\text{Pr}_x):\text{Ba}:\text{Cu}$ of 1:9:24. Then we place the mixture in a zirconia tray and heat it to 980°C, where it is held for an hour. Next, we lower the temperature at a rate of

6.2°C/h to 880°C and then at a rate of 100°C/h to room temperature. The resulting crystals are typically $1 \times 1 \times 0.003$ mm. The as-grown crystals are oxygen deficient and must be annealed in flowing O_2 at 420°C for seven days.

Figure 1 shows the electrical resistivity as a function of temperature for a series of crystals grown with this technique. We used an electron microprobe to determine the praseodymium concentration of the crystals. These results show that the values of $T_c(x)$ for the crystals grown in zirconia are consistent with the results from polycrystalline samples.

When shock-compacting single crystals, we found that the incident shock wave tended to break the crystals into many tiny pieces. Because we wanted to preserve the integrity of the crystal for laboratory characterization and minimize the effects of grain boundaries, we performed preliminary studies on single crystals of $YBa_2Cu_3O_{7-\delta}$ using different mounting techniques. We varied the angle of incidence between the crystal and the impactor and changed the applied shock pressure. Shock pressure was applied using a two-stage light-gas gun.

Our results suggest that a specimen angle of 30 deg between the normal angle to the single-crystal specimen and the shock wave and a shock pressure of about 2.5 GPa (25 kbar) or greater should minimize the damage to the crystal and induce enough structural defects to increase the flux-pinning energy and the critical current density. We characterized preshocked crystals using magnetic relaxation and hysteresis measurements and are preparing them for shock compaction.

Figure 1. Normalized electrical resistance as a function of temperature for a series of $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$ single crystals. These results show that the values of $T_c(x)$ for the crystals grown in zirconia are consistent with the results from polycrystalline samples.

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1. Weir, S. T., W. J. Nellis, C. L. Seaman, E. A. Early, M. B. Maple, M. J. Kramer, Y. Syono, M. Kituchi, P. C. McCandless, and W. F. Brocious (1992), "Shock Compaction of High- T_c Superconductors," in *Shock-Wave and High-Strain-Rate Phenomena in Materials*, M. A. Meyers, L. E. Murr, and K. P. Staudhammer, Eds. (Marcel Dekker, New York, NY), p. 759.

References

Commissioning the High-Pressure Crystallography Diffraction Station of UC–LLNL Beamline 10–2 at SSRL

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

LLNL Collaborator: Marvin J. Weber

Students: Mike Chan, Hyunchae Cynn, Douglas Gibson, Richard Jacobinas, Amy Martin, and Susanna Mustonen (UC Los Angeles)

Abstract

We are commissioning and testing the x-ray diffraction station on beamline 10–2 at UC's X-Ray Standards and Calibration Facility (XCSF) at the Stanford Synchrotron Radiation Laboratory (SSRL). The XCSF consists of state-of-the-art beamlines and experimental stations at SSRL and the National Synchrotron Light Source, which were constructed by a UC–National Laboratories Participating Research Team (PRT) with funds from the Department of Energy, LLNL, the UC President's Office, and most of the UC campuses. The XCSF was built to enhance UC's capacity for research with vacuum ultraviolet and x radiation in biology, chemistry, earth sciences, engineering, materials science, and physics. During FY 1992, we obtained the first high-pressure x-ray diffraction patterns with this facility on samples of nickel, sulfur, and EuCo_2P_2 .

Objectives

Scientists believe that the cores of the Earth and the terrestrial planets contain a large proportion of iron. Other important elements may include nickel, oxygen, sulfur, and silicon. More primitive planets, their satellites, and comets are believed to be composed of dense, often hot mixtures of relatively simple molecules. We want to determine the pressure, specific volume, and temperature (P - V - T) equations of state for these materials at high pressures and high temperatures to constrain models of the interiors of these bodies. Measurements of the equations of state at high static pressures (and eventually high temperatures) would be useful for connecting the shock- and static-compression data and for testing the accuracy of models used to extrapolate from laboratory to core conditions.

The diffractometer we are installing is designed to gather such P - V - T data at static high pressures and high temperatures using diamond-anvil cells, thus allowing us to measure temperature, pressure, density, electrical resistivity, and x-ray diffraction patterns of samples in situ. A major limitation for diffraction experiments with these techniques has been the intensity of available sources. The PRT's new system at SSRL overcomes many of these limitations.

The XCSF at SSRL consists of two beamlines and three experimental stations built by scientists and engineers from several UC campuses and LLNL. These beamlines are world-class facilities for research with vacuum ultraviolet and soft- and hard-x-ray radiation. At the start of this project, the beamline facilities were complete except for installing the diffractometer at the hard-x-ray station of beamline 10–2. Our objectives were to install several components of the diffractometer, including the goniometer, drive motors, slits, detectors, positioning table, and sample holders, and to make the first high-pressure studies with the system.

The diffractometer and most of the related components arrived at SSRL during the fall of 1991. Soon thereafter, we began installing the components and were assisted by the SSRL staff and Phil Wade, the PRT technician. We tested the hardware during a three-day shakedown run in the spring of 1992. The capabilities of the system and detectors were demonstrated during an eight-day run in July.

The benefits of the flexible motorized positioning system were immediately apparent. After sample changes, we could align the system within several minutes in the best case and within an hour in the worst case. Especially good success was demonstrated using image plate collection techniques with nickel, the photophase of sulfur, and a sample of EuCo_2P_2 provided by a group at UC Berkeley. We collected good diffraction patterns at high pressures with exposure times of 5 to 40 min. Programs to analyze the 11-Mbyte diffraction pattern files collected with image plates are being written at UC Los Angeles. We also tested the Ge(Li) detector and a position-sensitive detector at UC Berkeley. We will continue the experimental work during SSRL's 1993 operating period.

After initial experiments to demonstrate the sensitivity of the apparatus, we plan to study two systems for which work has been limited by problems associated with conventional sources. First, we will study the structure of $\epsilon\text{-O}_2$. Although a satisfactory monoclinic unit cell has been defined, the positional parameters of the inequivalent molecules could not be determined because of weak intensities. The second system is sulfur for which we want to characterize a new, high-pressure phase that was established in the UC Los Angeles laboratory. Preliminary experiments with a Rigaku rotating-anode source and several-day exposures yielded only a weak powder pattern.

A New Apparatus for Measuring the Thermal Expansivity of Minerals at High Temperatures

Principal Investigator: Orson L. Anderson (UC Los Angeles)

LLNL Collaborator: David J. Erskine

Abstract

A state-of-the-art interferometer has been constructed at the Mineral Physics Laboratory at UC Los Angeles. This interferometer is the basis of a new measurement technique for thermal expansivity at very high temperatures. Our principal goal is to improve the accuracy of measurements of length change. In FY 1992, we concentrated on automating the experiment with a computer control system and on installing the required optical components.

Objectives

We want to accurately measure the thermal expansivity of minerals at temperatures up to 2000 K so that we can develop reliable equations of state for mantle materials at mantle conditions.¹ Current measurements of insulators are limited to about 1300 to 1500 K with large errors at the upper temperatures. Because of these errors, extrapolation to temperatures up to 2000 K is uncertain. Therefore, we have built an experimental apparatus for measuring the thermal expansivity of silicates to temperatures of 2000 K using the principles of optical interferometry and a helium–neon laser.

In FY 1992, we built an interferometer that eliminates the unwanted effects of building vibration room lighting and of sample incandescence. When the sample expands thermally, the change in length is detected by the interferometer with a spatial resolution of about 10 nm. The interferometer measures the difference in optical path lengths between the two parallel top and bottom sides of the sample and subtracts the unwanted portion of the signals. This feature is called push–pull because it uses the outputs of the interferometer in differential mode. The design is based on principles used to measure velocity histories.² During FY 1992, we incorporated the required optical components into the system and installed a computer control system.

Progress

The interferometer has four optical outputs; pairs of the outputs are summed electronically to yield two fringe outputs. When the fringe outputs are arranged 90 deg out of phase, the direction of sample motion can be determined. The sample length normally increases with increasing temperature, although anomalous phase transformations can cause the opposite effect. The locus of angular motion detected by the interferometer yields the expansion of the sample.

During FY 1992, we designed and installed the required optical components and put a computer control system into operation. We installed a piezoelectric transducer to calibrate the interferometer against preselected length changes. With this transducer, we can obtain a given length change of a representative order of magnitude by applying a given increment of applied voltage.

The basic interferometer has been successful. Further research is needed to improve the spatial resolution and to obtain a high-temperature furnace with minimal effects of thermal convection.

References

1. Anderson, O. L. (1991), "Accurate Thermal Expansivity Measurements in the Range 1500–2000 K Are Needed for Minerals," *Int. J. Thermophys.* **12**, 757.
2. Hemsing W. F. (1979), "Velocity Sensing Interferometry," *Rev. Sci. Instrum.* **50**, 73.

Astrophysics

Optical Properties of Nearby Radio Galaxies

Principal Investigator: Hyron Spinrad (UC Berkeley)

LLNL Collaborator: Willem van Breugel

Student: Arjun Dey (UC Berkeley)

We have almost completed the observational aspects of our project to study possible relations between the radio and optical properties of a complete sample of powerful, low-redshift radio galaxies. Several galaxies in our sample show extended ultraviolet (UV) continuum-emitting regions that in many instances are associated with the extended radio structure. In some instances, the physical processes responsible for the UV emission are due to star formation; in others, they are due to non-thermal processes such as synchrotron emission or to scattering. We are analyzing the data in detail and plan to finish this project in FY 1993.

Abstract

The question of how galaxies evolve is one of the fundamental problems in modern astronomy. Galaxy samples selected by radio flux have thus far been the most successful in helping us find objects that may belong to the same parent population over a large redshift range. As a result, a large fraction of what we know about galaxy evolution over a large redshift range is based on the study of radio galaxies. One of the most interesting discoveries in radio galaxy research in the last decade is that high-redshift galaxies ($z \geq 0.7$) show extended UV (and sometimes optical) continuum emission that is aligned with the nonthermal radio continuum emission. This alignment effect is generally attributed to star formation triggered by radio lobes passing through a dense ambient medium. However, high signal-to-noise moderate-resolution spectra of the continuum light are difficult to obtain, and optical polarization has been detected in some high-redshift radio galaxies. Therefore, we cannot rule out other physical processes, such as scattering, that may be responsible for the alignment of the optical and UV continua. As a result, we are imaging a well-defined sample of nearby radio galaxies to identify similar alignment effects between the radio and the UV continuum emission. Since these low-redshift objects are optically much brighter than their high-redshift counterparts, they can be studied in greater detail. Thus, we hope we can identify the dominant physical process that may be responsible for the alignment effect seen in high-redshift radio galaxies.

Objectives

During FY 1992, we obtained a large fraction of the imaging and spectroscopic data for this project. The data were obtained at the 3-m Shane telescope at the Lick Observatory, the 1.5- and 4-m telescopes at the Cerro Tololo Inter-American Observatory, the 2.1-m telescope at the Kitt Peak National Observatory, and the 3.6-m telescope at the European Southern Observatory. Our sample consists of 54 radio galaxies selected from the 3CR and PKS radio catalogs on the basis of their redshifts ($0.079 < z < 0.2$ for 3CR, and $0.1 < z < 0.2$ for PKS). We constructed special filters to image these galaxies in their continuum light in the near UV and in the red and to minimize the contamination from strong emission lines.

Progress

Thus far, we have imaged about 78% of the sample and are analyzing the data. About one-third of the objects imaged show bright, extended UV continuum emission, which appears to be associated with the nonthermal radio continuum emission. In some cases, the host galaxy itself has extended UV continuum emission that is spatially distributed differently from the red continuum. If the UV continuum emission is due to starlight, this would be strong evidence for enhanced star formation associated with the radio source. In other cases, extended UV continuum emission is found at large distances from the host galaxy (tens of kiloparsecs) but still appears to be associated with the radio source (Figure 1). In the cases studied spectroscopically thus far, these extended UV continuum-emitting regions have strong associated line emission and are at the same redshift as the host galaxy of the radio source. In at least one case, the line emission and UV continuum emission appear to be due to starlight. In other cases, the emission line spectrum is similar to the spectra seen in the emission line filaments in Cen A. These objects will be of great assistance in studying the interaction of the radio source with ambient medium and in probing the nucleus of the host galaxy of the radio source. Our images will also be useful for studying the environments of the nearby radio sources.

Nearby radio sources also show evidence that their environments are affected by the presence of the radio source. Therefore, they provide good laboratories for studying the environmental effect of an active nucleus. In a related study, we are investigating the stellar and gaseous content of a sample of gas-rich galaxies that contain radio sources. This sample was defined by cross-correlating the University of Texas 365-MHz radio catalogs with the Infrared Astronomy Satellite (IRAS) Faint Source Survey database. We also obtained optical broadband images at the Very Large Array (VLA) radio telescope. We discovered that some of the

Figure 1. A 1.4-GHz radio map from the VLA radio telescope at 1.5 arcsec overlaid on a grayscale of the R-band image of 3C 285. The object labeled 9.6 is located 45 arcsec (61 kpc in projection for a Hubble constant $H_0 = 75 \text{ km} \cdot \text{s}^{-1} \cdot \text{Mpc}^{-1}$ and a deceleration parameter $q_0 = 0.5$) from the nucleus of 3C 285 and is at the same redshift as 3C 285. In addition, it has an HII-region spectrum, colors indicative of a young stellar population, and shows an edge-brightened morphology in its H α line emission and UV continuum, which supports the hypothesis that 9.6 is a starburst triggered by the radio source.

Texas-IRAS sources have optical spectra that show emission lines characteristic of photoionization by an active galactic nuclei (AGN) in addition to Balmer absorption lines, which are generally interpreted as evidence for a recent episode of star formation. This finding provides further circumstantial evidence that the presence of an active nucleus is somehow related to the stellar evolutionary history of the galaxy. The objects that we discovered are important for studying the starburst-AGN connection.

Synthetic Spectra of Supernovae: Comparison with Observations

Principal Investigator: Alexei V. Filippenko (UC Berkeley)

LLNL Collaborators: Samuel Dalhed and Thomas Weaver

Students: Thomas Matheson and Michael Richmond (UC Berkeley)

Abstract

We have acquired and are reducing the data on new spectra of supernovae. Although we obtained data on many supernovae, thus far we have focused our attention on two exciting objects: SN 1991T in NGC 4527 and SN 1991bg in NGC 4374. Both objects are Type Ia supernovae, but they exhibit striking peculiarities. We showed that SN 1991T may have been anomalously luminous compared with normal Type Ia supernovae and that SN 1991bg was definitely subluminous. Our study demonstrates that not all white dwarfs explode in exactly the same manner, so Type Ia supernovae must be used with caution as standard candles for determining the distances of galaxies. We made progress on modeling the supernova spectra in two key areas: (1) We improved a computer code that will perform the time- and space-dependent evolution of the radiation field in a manner that is consistent with the ionization state of the matter. (2) We developed atomic models for neutral and near-neutral iron.

Objectives

We obtained high-quality optical spectra and light curves of several supernovae for as long a time interval as possible (up to one year). Preliminary, rather qualitative inferences were drawn from a coarse analysis of the data. However, not much detailed theoretical modeling of the long-term spectral evolution of supernovae has been done anywhere in the world; thus, our knowledge of the physical conditions in the ejecta (such as chemical composition and temperature) is incomplete, so we cannot fully understand the explosion mechanism. This problem occurs in part because of the amount of time required to develop and run satisfactory numerical codes for different types of supernovae. Even where a synthetic spectrum is already available from another group, we must compare the results with those obtained from a different, independent code. The computations are complex and may be sensitive to minor changes in the assumptions used.

Scientists at LLNL have been working on theoretical models of supernovae for several years and have the expertise to produce realistic synthetic spectra of supernovae. Sam Dalhed developed a state-of-the-art radiation transfer code that can be modified for supernova atmospheres, and Thomas Weaver has new, realistic models for supernova explosions. Our objective in this project was to compare the high-quality optical spectra with the synthetic spectra produced by the modified radiation transfer code, so we can better understand the explosion mechanisms and ejecta of supernovae.

Progress

SN 1991T. The premaximum spectrum of SN 1991T did not resemble that of any known supernova. It seems to have been dominated by lines of iron-group elements, although we will not be certain until we construct synthetic spectra with the radiation transfer code.¹ Near the maximum brightness, however, lines of intermediate mass elements slowly appeared. With time, the spectral similarity to classic Type Ia supernovae grew progressively stronger. We believe that, two months after the explosion, the spectrum was again dominated by iron-group elements, and it

appeared almost identical to that of typical Type Ia supernovae. At visual wavelengths, SN 1991T may have been ≥ 0.6 magnitude more luminous than classical Type Ia supernovae. These properties suggest that SN 1991T may be the result of a double detonation of a white dwarf, initiated at the boundary layer between the C–O core and the helium envelope. Alternatively, the explosion may be the result of a delayed detonation in a C–O white dwarf.

To test the detonation hypothesis, we plan to compare Dalhed's synthetic spectra with the observations. We initially measured the strengths, velocity widths, and observed wavelengths of the absorption lines in the early-time spectra to use as a guide. Some evidence appears for doubly ionized iron or perhaps even nickel; if correct, this evidence provides partial support for the detonation model. However, the detonation model makes some fairly strong predictions about the late-time spectrum, as discussed by Axelrod.² Thus, during FY 1992, we obtained late-time spectra of SN 1991T. We are reducing and analyzing the data, and the results will be of direct relevance to Dalhed's calculations. Preliminary comparisons suggest that the late-time spectrum of SN 1991T does not greatly differ from that of normal Type Ia supernovae. If this result is confirmed, we will probably focus on spectral synthesis in the context of deflagration models rather than detonation models.

SN 1991bg. One of our other main targets during this project was SN 1991bg, a peculiar Type Ia supernova located in the outskirts of the E1 galaxy NGC 4374 (M84, in the Virgo cluster). This object was discovered in December 1991, and Filippenko et al. described the initial data set.³

At maximum brightness, SN 1991bg was 2 to 3 magnitude subluminous at optical wavelengths, compared with normal Type Ia supernovae. Although it was very red, it did not appear significantly reddened by interstellar dust. The decline from maximum was much faster than normal. Despite having prominent Si–II absorption near 615 nm, characteristic of Type Ia supernovae, SN 1991bg was spectroscopically peculiar at maximum brightness; a deep trough was present around 420 nm. Spectral synthesis by David Branch suggests that this feature is produced by singly ionized titanium, but those results should be checked with an independent code such as Dalhed's radiation transport code.

Lines due to other intermediate-mass elements were also strong near maximum brightness, but the expansion velocity (about 10,000 km/s) was somewhat lower than the average velocity, which is about 11,000 to 13,000 km/s for Type Ia supernovae. Also, three weeks past the maximum brightness, the spectrum in certain respects more closely resembled spectra of Type Ib or Ic than of Type Ia supernovae. These properties suggest that SN 1991bg was produced by the slow deflagration of a white dwarf. The observed expansion velocities, however, are too large unless a sub-Chandrasekhar mass of material was ejected. An unusually low mass for the ejecta, expanding at a nearly normal velocity, is consistent with the observed early transition to the nebular phase and with the rapid brightness decline. Thus, SN 1991bg may have resulted from the deflagration of an outer layer of material on top of a C–O core or perhaps from the explosion of a low-mass white dwarf.

Theoretical models. We made progress on modeling the supernova spectra in two key areas. The first is in connection with a simulation code known as GLF. This code will perform the time- and space-dependent evolution of the radiation field in a manner that is consistent with the ionization state of the matter. During FY 1992, we made several improvements throughout the code and upgraded the radiation transport package so it can handle any number of interlocking lines using the complete linearization method. We also implemented and tested the interaction of the line radiation with the continuum. We have not added the interaction of the Compton electrons, which exist in addition to the thermal background electrons, in the full code. However, we have extracted the necessary portions of the code and

are experimenting with multicomponent electron distribution functions. These electrons, balanced by radiative recombination, drive the ionization balance in Type I supernovae.

The second area of progress is in developing atomic models for neutral and near-neutral iron. We generated a rather large base model, which contains radiative rates calculated using relativistic Hartree–Slater methods, Dirac single-shell photoionization rates, and Coulomb–Born exchange electron collisional cross sections. Then we modified the model to use state-to-state photoionization cross sections rather than shell-averaged values. In this context, we adapted a locally written (unpublished) set of codes that takes the wave functions generated by the GRASP code, calculates the coupling coefficients, and produces the correct state-to-state photoionization cross sections. Since the base code contains approximately 10,500 energy levels and 350,000 lines of data, we averaged it down to be of practical use.

We also modified the GRASP atomic structure package of Ian Grant to provide detailed, fully relativistic, multiconfigurational radiative transition rates. The wave functions generated are fed into a distorted-wave collisional cross-section code for high-quality cross sections. To check the accuracy of the single-channel distorted-wave cross sections, we obtained the structure and cross-section codes called RMATRIX, which use the close-coupling approach to collisional cross sections.

References

1. Filippenko, A. V., M. R. Richmond, T. Matheson, J. C. Shield, E. M. Burbidge, R. D. Cohen, M. Dickinson, M. A. Malkan, B. Nelson, J. Pietz, D. Schlegel, P. Schmeer, H. Spinrad, C. C. Steidel, H. D. Tran, and W. Wren (1992), “The Peculiar Type Ia SN 1991T: Detonation of a White Dwarf?” *Astrophys. J. Lett.* **384**, L15.
2. Axelrod, T. (1980), *Late-Time Optical Spectra from the ^{56}Ni Model for Type I Supernovae*, Ph.D. thesis, University of California at Santa Cruz.
3. Filippenko, A. V., M. R. Richmond, D. Branch, C. M. Gaskell, W. Herbst, C. H. Ford, R. R. Treffers, T. Matheson, L. C. Ho, A. Dey, W. L. W. Sargent, T. A. Small, and W. J. M. van Breugel (1992), “The Subluminous, Spectroscopically Peculiar Type Ia Supernova 1991bg in the Elliptical Galaxy NGC 4374,” *Astron. J.* **104**, 1543.

Cosmic Structure Formation Seeded by Global Monopoles and Textures

Principal Investigator: Lars Hernquist (UC Santa Cruz)

LLNL Collaborator: David Bennett

In this project, we are studying a class of models for generating the primordial density fluctuations that have grown by gravitational instability to form the galaxies and large-scale structure that we observe in the universe today.

Abstract

Our models indicate that the primordial density fluctuations are the remnants of a phase transition that occurred very early in the history of the universe when the temperature was about 1016 GeV. If such a phase transition led to the spontaneous breaking of a global symmetry, the field that underwent the symmetry breaking can only begin to correlate itself on scales inside the horizon at subsequent times (barring a late round of inflationary expansion). The dynamics of this field as it tries to smooth itself out on the horizon scales can lead to the annihilation of topologically nontrivial entities known as global monopoles or cosmic textures, depending on the details of the field theory. Generally, however, the dynamics of this field will produce gravitational perturbations with about the right amplitude to induce galaxy formation. Our goal in this project was to model the development of the gravitational perturbations.

Objectives

The study of theoretical models for cosmic structure formation was transformed by the discovery of anisotropies in the cosmic microwave background radiation announced by the Cosmic Background Explorer (COBE) Differential Microwave Radiometer experiment in April 1992. These anisotropies can be considered to be a measure of primordial gravitational perturbations. With them, we can pin down the amplitude of the perturbations much better than we can with measurements of galaxy distributions, which include uncertainties in the process of galaxy formation. The COBE detection put the anisotropies at a level somewhat higher than predicted by the most conventional models in which the gravitational fluctuations are generated by inflation. The higher level is encouraging for proponents of topological defect models such as global monopoles and textures, which predict a higher ratio of microwave background fluctuations to density perturbations than does inflation.

In fact, low-resolution gravitational n -body simulations indicate that the global monopole and texture models work well with the COBE normalization, but with a catch. To fit the COBE normalization, we must assume that the perturbation amplitude is somewhat lower than is normally assumed. This lower amplitude actually improves many of the observational tests done by Bennett et al.; however, there may be a flaw in this analysis that results from the low resolution of the simulations. The question is whether this low amplitude is sufficient to allow galaxies to form at a reasonable redshift.

To address this question, we refocused our high-resolution calculations to study the low-amplitude, or high-bias, global monopole and texture seeded galaxy formation scenarios. We performed several n -body calculations using hierarchical tree code, which enables us to use large numbers, typically several hundred thousand

Progress

particles, and simultaneously resolve scales comparable to those thought characteristic of dark matter halos surrounding typical galaxies. We are analyzing our simulations to determine if these scenarios can form a structure on a galaxy scale similar to those that were observed and at the same time, satisfy the constraints on large scales imposed by the COBE results.

Relativistic Shock Waves and the Excitation of the Crab Nebula

Principal Investigator: Jonathan Arons (UC Berkeley)

LLNL Collaborators: A. Bruce Langdon, Claire E. Max, and Marco Tavani

Student: Yves Gallant (UC Berkeley)

Abstract

In this project, we used the results of previous particle-in-cell simulations of plasma shock waves to predict the nebular synchrotron emission from the binary pulsar of PSR 1957+20. We also used these results with a semianalytical model of the relativistic shock structure, which is designed to give a quantitative theory of the wisps in the synchrotron emission of the Crab Nebula. These wisps are the principal observational manifestation of the shock that terminates the wind from the Crab pulsar. We found that the magnetic fields of millisecond pulsars are largely dipolar. Also, during FY 1992, we successfully migrated the particle-in-cell code ZOHAR to work on ordinary workstations and other easily accessible computers.

Objectives

In this project, we are trying to understand the origin of nonthermal energy in astrophysical sources of synchrotron radiation. Our goal was to apply the physics of relativistic shock waves to the origin of synchrotron emission in supernova remnants powered by pulsars, especially to the Crab Nebula, and to hypothesized nebular synchrotron emission from the binary pulsar PSR 1957+20. We also wanted to convert the basic particle-in-cell code ZOHAR to a form that could be used in LLNL's Open Computing Facility and elsewhere.

Progress

With the support of previous grants, we used particle-in-cell computer simulations and linear instability theory to investigate collisionless, relativistic magnetosonic shock waves in plasmas that are composed of electrons and positrons and that are polluted by heavy ions whose number density is smaller than that of the pairs. We found that when the heavy-ion population contains most of the upstream kinetic energy, a large fraction of the flow energy is fed into a nonthermal distribution of pairs. This distribution is Maxwellian at low energy but is a power law at high energy, with a power-law slope in the right range to explain the synchrotron spectra observed in nonthermal radio sources powered by relativistic winds. The mechanism of energy transfer is synchrotron maser emission of magnetosonic waves by the ions, which gyrate quasi-coherently in the magnetic field of the shock front. These left-elliptically polarized waves are resonantly absorbed by the pairs. The efficiency of this acceleration process can approach 20%.

Qualitative applications of this process to models of the inner region of the Crab Nebula suggest that the pulsar loses most of its energy in a flow of partially ionized iron ions with energy on the order of 100 peV/ion. We suggested that optical observations spatially resolve the shock structure and that the wisps in the nebular emission are the regions of strongest magnetic field within the shock structure. These computational models are for plane parallel shocks. However, to apply them to the Crab Nebula, we must incorporate the expanding geometry of a quasi-spherical outflow.

During FY 1992, we constructed a semianalytical theory of the shock structure, which will allow us to model the spatial structure of the shock so we can compare the model to observations. Hoshino et al. correlated the compressions in the magnetic field induced by the gyrating heavy ions with the observed wisps in the Crab Nebula.¹ These compressions are narrow bands of enhanced surface brightness, located spatially where the pulsar's wind should terminate in a shock wave as indicated by ideal flow solutions. The basic theoretical idea is to represent the ions as a cold stream, reflected and gyrating in the increasing magnetic field of the shock front and embedded in pairs already heated by a pure pair shock that lies at the leading edge of the structure. In essence, this is a solitary wave model, since ion dissipation is (so far) neglected, including the effects of charge separation between the ions and the pairs and the effects of spherical expansion.

In our models, a solution is constructed by guessing the magnetic field structure, integrating the ion orbit equations in that structure, then using the results to construct the ion current and charge densities. These results are added to the current densities and charge densities of the pairs, treated as a small Larmor radius fluid. These sources are used in the Ampere and Coulomb equations to find a new iterate for the fields, and the procedure continues until convergence is achieved. Figure 1

Figure 1. Transverse magnetic field (solid curve) and electric field (dashed curve) of the ion soliton model of shock structure as a function of radius from the pulsar, measured in units of r_1 , the radius where the pairs are shock-heated at the leading edge of the structure. We assumed that flow in the shock frame is steady. Peaks occur at each turning point, where the gyrating ion stream reverses direction in the magnetic field, whose presence supports the outflow. The parameters are for a structure that is more strongly magnetized upstream than the final model will be. As a result, the strength of the field just behind the shock in the pairs is 1.1 times the strength of the field in the upstream flow.

shows a preliminary example of such a structure, illustrating that spherical divergence of the shock structure weakens the amplitude of the magnetic compressions with radius, a result qualitatively in accord with the observed dimming of the wisps with radius. We will complete this model in FY 1993 and compare it to the observations of the wisps' surface brightness.

We also applied the results from the shock studies to predict x- and gamma-ray emission from millisecond pulsars in close binaries. One pulsar we studied is PSR 1957+20, a curious system in which the energy from the pulsar is causing the ordinary star to evaporate. In contrast to diffuse systems such as the Crab Nebula, the accelerated particles within the binary lose energy to synchrotron emission as fast as they gain it, because of the much stronger magnetic field present within the binary's close quarters. We calculated the fluxes expected at the Earth and showed that the Gamma-Ray Observatory might be able to detect this system, but only if unusually long observations are made.

In studying the observational constraints on the morphology of the pulsars' magnetic fields, we found that the spin-up of millisecond pulsars can occur as observed only if the magnetic fields of such old pulsars are basically dipolar, with no more than 40% pollution by large-scale anomalies such as quadrupole fields.

We also are converting our basic plasma simulation tool, the fully relativistic code ZOHAR, into a form that can run in LLNL's Open Computing Facility. With the support of the Plasma Physics Research Institute, the code has been used on a conventional SPARCstation to begin work on two-dimensional effects in the pairs contained in the relativistic shocks that terminate pulsar winds.

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1. Hoshino, M., J. Arons, Y. Gallant, and A. B. Langdon (1992), "Relativistic Magnetosonic Shock Waves in Synchrotron Sources: Shock Structure and Non-Thermal Acceleration of Positrons," *Astrophys. J.* **390**, 454.

References

Heavy-Element Nucleosynthesis in Massive Stars and Supernovae

Principal Investigator: Stanford Woosley (UC Santa Cruz)

LLNL Collaborators: Grant J. Mathews and William M. Howard

Student: Robert D. Hoffman (UC Santa Cruz)

Abstract

We have modeled the detailed nucleosynthesis that arises from the neutron-rich, α -particle-rich freeze-out of material that is initially in nuclear statistical equilibrium within the high-entropy wind of a young (1- to 10-s-old) neutron star in which neutrino energy deposition is driving mass loss. Rapid freeze-out in the presence of excess free neutrons allows heavy elements to synthesize above the iron group. In the limit of a very large fraction of unassembled α -particles and a large neutron excess, the α -process merges smoothly into the classical r-process. Such conditions occur naturally within the high-entropy evacuated region that comes to exist between the surface of a young neutron star and the outgoing shock within a Type II or Type Ib supernova, as are observed in the Wilson delayed explosion model. These conditions may exist in other regions as well.

A similar wind may also blow from the surface of a white dwarf during accretion-induced collapse to a neutron star, although the nucleosynthesis will be much different because the star has no overlying mantle. This mantle is necessary (in a Type II event) to tamp the explosion and provide, over several seconds, the requisite temperatures and densities needed to complete the r-process.

Objectives

We proposed to study several topics in stellar nucleosynthesis: (1) nucleosynthesis in the hot bubble relating to the high-entropy region that comes to exist between the surface of a young (1- to 10-s-old) neutron star and the receding accretion shock following core bounce within Type II or Type Ib supernovae; (2) accretion-induced collapse, in which a neutrino wind blows from a white dwarf after the dwarf collapses directly to a neutron star through slow accretion with little or no accompanying optical emission; (3) the p-process, which considers the production of proton-rich isotopes synthesized during convective oxygen burning in a massive star in hydrostatic equilibrium; (4) the s-process; and (5) explosive nucleosynthesis that covers the entire spectrum of explosive processing of material previously created by hydrostatic burning prior to core collapse in massive stars.

Progress

Nucleosynthesis in the hot bubble. Although preliminary results on the α -process and the r-process were accepted for publication in July 1991, we revised our work after conversations with Al Cameron, who pointed out a major deficiency in our reaction network. Specifically, we had neglected the reaction ${}^4\text{He}(\alpha, \gamma){}^9\text{Be}$. Subsequently, we devoted our research efforts during the first six months of FY 1992 to reinvestigating these two processes.¹

Our reaction network allowed us to track the evolution of the r-process only up to the point of charged-particle freeze-out. However, we can determine if a successful r-process will arise from a given calculation by observing the final neutron-to-seed ratio. In FY 1992, we showed that the model of Mayle and Wilson was inadequate to produce the conditions necessary to account for the solar r-process abundances. However, with small variations in certain critical parameters (entropy,

expansion timescale, and neutron excess), Meyer et al. showed that agreement with the solar r-process abundances could be achieved.² Figure 1 shows the solar-system r-process abundances (points) compared with the calculated averaged r-process abundances (solid line) of Meyer et al. weighted by $e^{-3\eta}$, where η is the initial neutron excess. The abundance curve is normalized to the solar-system r-process peak at ^{130}Te .

Using Wilson's most recent $20-M_{\odot}$ delayed explosion model, we carried out a set of parameterized calculations similar to those of Woosley and Hoffman¹ for a time 7 s after bounce. A time history for the temperature and density of a blob of material in a steady state was created from the temperature, density, and velocity data (as a function of mass) from Wilson's model and followed for temperatures between 1000 and 100 keV. Table 1 shows the results for variations of the entropy, initial neutron excess (where $\eta = 1 - 2Y_e$ and Y_e = electron fraction), and expansion timescale in terms of the final neutron-to-seed ratio and the final neutron and α -particle mass fractions.

The most sensitive parameter is the entropy (density), followed by the expansion timescale, and the neutron excess. A value of 100 neutrons per seed is required to build the mass 192 peak in the solar r-process abundance set. There are regions within Wilson's model in which $\eta = 0.16$ and regions in which the entropy is nearly 450. However, these regions occur at later times when the mass-loss rate is appreciably

Figure 1. The solar-system r-process abundances (points) compared with the calculated averaged r-process abundances (solid line) of Meyer et al., weighted by $e^{-3\eta}$, where η is the initial neutron excess. The abundance curve is normalized to the solar-system r-process peak at ^{130}Te .

lower ($M \leq 10^{-6} M_{\odot} \cdot \text{s}^{-1}$), thus leading to an inadequate r-process abundance yield. Although we have yet to calculate the r-process abundances resulting from these freeze-out calculations, we believe convergence toward the optimum conditions for a successful r-process can be obtained within the uncertainties of the Wilson model.

We will continue to emphasize the r-process within the Wilson explosion model. We are developing an abbreviated network of 10 isotopes that will more accurately track the reassembly of α -particles and nucleons into heavy elements during the freeze-out (at present, the Wilson code has no such provision). We estimate that this reassembly may enhance the entropy throughout the interesting regions of Wilson's model by about 5 to 10%. Additionally, we will drop the steady-state approximation to the wind by interpolating the time-dependent temperature and density in finely edited regions within Wilson's model.

Results from remeasuring the crucial ${}^9\text{Be}(\alpha, n){}^{12}\text{C}$ reaction rate³ indicate a 20% reduction for the rate over the temperature range of interest. This change will decrease the amount of α -particles reassembled during the freeze-out, causing all of the available neutrons to be incorporated into a smaller number of heavy nuclei. In the end, all of these may fail to give the necessary entropy, which thus will indicate new physics (additional heating at late times).

Accretion-induced collapse. We also studied the collapse of a white dwarf directly to a neutron star during slow accretion.^{4,1} As the white dwarf collapses, the neutrino energy is deposited into the atmosphere of the collapsing star, causing a super-Eddington luminosity to develop. A wind much like that in the Type II hot bubble can blow from the surface of the newly formed neutron star. However, because of the lack of an overlying massive star mantle, the mass-loss rate is much lower, and the material that has been subjected to the high density experiences very rapid neutron capture. We found that the resulting nucleosynthesis consists of heavy neutron-rich species whose production severely constrains the number of these events that could have taken place in our galaxy. Also, graduate student Frank Timmes and Woosley explored the conditions necessary to give collapse in accreting C–O and Ne–O white dwarfs.

During FY 1992, we revised our nuclear database to include many new experimentally determined reactions on proton-rich nuclei and to replace many approximations to reaction rates on unstable targets with detailed Hauser–Feshbach results from Thielemann⁶ for nuclei with $Z \leq \text{Kr}$. We are preparing a new compilation of our entire reaction database, which will tabulate all of our reaction rate information for strong, electromagnetic, weak, and neutrino-induced reactions. This is a major

Table 1. Results of parameterized nucleosynthesis.

Entropy	Initial neutron excess	Expansion time (s)	Neutrons/seed	Final mass fraction Neutron	α -particle
380	0.10	1.04	19	0.037	0.772
380	0.16	1.04	33	0.080	0.68
380	0.10	0.52	55	0.064	0.802
380	0.16	0.52	79	0.115	0.739
570	0.10	1.04	100	0.070	0.860

update to a widely cited unpublished work⁵ and will be a useful source of information for nucleosynthesis research. We are now ready to begin the p-process, s-process, and parameterized explosive nucleosynthesis studies with a network that we believe is the most up-to-date version available. For the p-process, we will perform a parameterized survey of simple two-zone model calculations to study the evolution of material that is mixed over a convective timescale under conditions appropriate to hydrostatic oxygen burning.

We completed the first series of stellar models over an extended mass range with variations in the $^{12}\text{C}(\alpha,\gamma)$ rate, semiconvection, mass zoning, and initial metallicity. The purpose of the runs was to distinguish the various subtleties in each mass star vs these parameters. The next series will produce the neutron exposure strengths as a function of the Lagrangian mass coordinate along with the temperature–density histories accompanying each exposure. These will form the basis of the s-process studies in future collaboration.

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1. Woosley, S. E., and R. D. Hoffman (1992), “The α -Process and the r-Process,” *Astrophys. J.* **395**, 202.
 2. Meyer, B., G. Mathews, W. M. Howard, S. E. Woosley, and R. D. Hoffman (1992), “r-Process Nucleosynthesis in the High-Entropy Supernova Bubble,” *Astrophys. J.* **399**, 656.
 3. Kavanaugh, R., and P. Wrean (1992), private communication.
 4. Woosley, S. E., and E. Baron (1992), “The Collapse of White Dwarfs to Neutron Stars,” *Astrophys. J.* **391**, 228.
 5. Woosley, S. E., and R. D. Hoffman (1986), “Tables of Reaction Rates for Nucleosynthesis ($6 \leq Z \leq 36$),” version 86.3, (unpublished).
 6. Thielemann, F. K., M. Arnould, and J. W. Truran (1987), *Advances in Nuclear Astrophysics*, eds. 525.

References

Toward Primordial Nucleosynthesis Constraints on the Dynamics of Cosmic QCD Phase Transition

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

LLNL Collaborators: Charles R. Alcock, David Dearborn, Robert Malaney, Grant J. Mathews, James R. Wilson, and Ron Mayle

Students: Karsten Jedamzik and Yongzhong Qian

Abstract

We used inhomogeneous primordial nucleosynthesis calculations to constrain the subhorizon-scale entropy fluctuations in the early universe. In these calculations, nuclear reactions are implicitly coupled with diffusive and hydrodynamic fluctuation-damping processes involving neutrinos, photons, and baryons. Our calculations and the primordial abundances of the light elements that are inferred from observation imply that only narrow ranges of fluctuation characteristics are acceptable. These ranges thus constrain the physics of the cosmic quantum chromodynamics and electroweak epochs that are unattainable by current terrestrial laboratory experiments.

Objectives

Prior to our work, calculations of inhomogeneous nucleosynthesis did not include several physical processes that are important for characterizing the nucleosynthesis produced by a given fluctuation. Entropy fluctuations produced in vacuum phase transitions at early epochs in the history of the universe are born with an isocurvature or isothermal character. They then experience rapid hydrodynamic expansion and evolve to a state in which they are in pressure equilibrium with their surroundings. Subsequently, they are damped by neutrino, photon, and baryon diffusion. These damping processes proceed through the nucleosynthesis epoch and can be effective on timescales that are comparable to the nuclear reaction timescales. We studied these processes in detail and produced the first primordial nucleosynthesis calculation to include all relevant effects.

Progress

In FY 1992, we accomplished all of our objectives. Our results indicate that the ${}^7\text{Li}$ abundance is the most severe constraint on entropy fluctuation characteristics and on the baryonic contribution to the closure density W_b . We found that the limit from homogeneous nucleosynthesis cannot be evaded for any fluctuation characteristics. Also, for low W_b , there are fluctuation parameters that are consistent with light-element abundances yet allow significant production of intermediate mass elements. We are extending our results to try to constrain the baryon number generating processes at the electroweak epoch.

In addition, during FY 1992, we studied the galactic chemical evolution of ${}^4\text{He}$ in light of primordial nucleosynthesis.¹ We also used primordial nucleosynthesis considerations to place limits on the magnetic moments of heavy neutrinos.²

References

1. Mathews, G. J., R. Boyd, and G. M. Fuller (in press), "Chemical Evolution of Irregular Galaxies and the Primordial ${}^4\text{He}$ Abundance," *Astrophys. J.*
2. Kawano, L. H., G. M. Fuller, R. A. Malaney, and M. J. Savage (1992), "Limits on Magnetic Moments of Heavy Neutrinos from Nucleosynthesis," *Phys. Lett. B* **275**, 487.

Spectral Models for Atmospheric Turbulence Effects on Large Telescopes

Principal Investigator: Stanley M. Flatte (UC Santa Cruz)

LLNL Collaborator: Claire E. Max

Student: L. William Bradford (UC Santa Cruz)

Investigations continue on the nature of the power spectrum of optical phase fluctuations caused by variations in the index of refraction arising from atmospheric turbulence. This work is directed at understanding how the standard model of atmospheric turbulence and possible deviations from that model will affect the performance of large optical telescopes and arrays of telescopes. Although the standard Kolmogorov model seems to work fairly well in accounting for most of the effects seen in astronomical observation, there are many exceptions, which require detailed modeling. The primary tool used in our analysis is a computer code that considers how fundamental quantities vary with altitude, including wind velocity, inner scale size, outer scale size, and C^2_n , the strength of variations in the index of refraction and the power law of the spectrum applicable at a given altitude.

Abstract

Our objective is to model the effect of atmospheric turbulence on optical propagation without assuming that the turbulence is characterized by homogenous, isotropic, Kolmogorov turbulence and using models that do not presume only the weak fluctuation limit. The method we chose is numerical simulation, in which a set of random phase screens is used to simulate the effects of atmospheric layering. Each layer can have a different strength, power-law index, inner scale, outer scale, and anisotropy. The simulations typically use up to 20 phase screens with a 512×512 grid size.

Objectives

To compare the simulation results with experimental data, we chose as a first data set the measurements of phase fluctuations collected by a group at the Space Sciences Laboratory (SSL) at UC Berkeley.¹ The issues raised by the SSL measurements include non-Kolmogorov slopes, differences between near-ground and high-altitude turbulence, and questions about the validity of the Taylor hypothesis. The phase-screen method provides a convenient format to simulate these effects: For example, it will simulate differences between the boundary layer (or the dome) turbulence and turbulence at a higher altitude. Using various model spectra, we can generate the phase and intensity variations that would be present at the entrance pupil to a single telescope or to an array of telescopes.

Continued literature searches and frequent communication with experimenters in astronomy and the atmospheric sciences have further improved our understanding of the current status of both theory and experiment. In addition, our simulations can produce results that agree with experimental results.

Progress

The SSL, UC Santa Cruz, and LLNL groups met several times to discuss the SSL data. We used calculations made with numerical-integration codes to model how variations in the outer scale affect the structure functions of phase and the Allan variance of phase. We found that some aspects of the SSL group's observations of non-Kolmogorov behavior of the structure function and Allan variance could be modeled with some assumptions about the outer scale. The most specific

assumption involved setting the outer scale equal to the separation of the two telescope elements. This assumption implies that somehow the finite baseline of the interferometer acted as the largest scale of turbulent fluctuations. However, the model used for these calculations was rather crude, so we believe the results are qualitative only.

Other results included deriving an expression for the Allan variance of phase for a two-element interferometer in terms of phase structure functions. We demonstrated that when the argument of the Allan variance corresponds to a spatial separation (by the Taylor hypothesis) that is larger than the optical path length in the interferometers, a power law exponent of $-4/3$ rather than $-1/3$ is expected. For the SSL experiment, this finding is relevant only for the measurements made with the He-Ne laser Doppler interferometers mounted on each telescope, not for the results obtained with the stellar observations, which have very long path lengths. However, these points do not change the results of the SSL experiment.

None of the calculations used a sufficiently detailed model to allow us to separate the contributions made by varying parts of the atmosphere. The necessity for this was recognized in the SSL group's report, where they attempted to identify the fractional contribution to the phase fluctuations from turbulence close to the ground.¹ Furthermore, numerous reports by astronomers indicate that effects from the boundary layer or from domes contribute significantly to "seeing" effects.²⁻⁴ The best technique for separating the different atmospheric contributions will apparently be to compare the data to results of the multiple-phase-screen numerical simulations.

Although results from many experiments other than the SSL experiment show non-Kolmogorov behavior, others experiments present results in good agreement with the Kolmogorov model.⁵⁻⁸ However, in the SSL experiment, many sources of turbulence can be identified. The trailers containing the telescopes are on the order of $13 \times 4 \times 3$ m and are separated by 4 or 13 m. The trailers act as sources of turbulent eddies, both from thermal convection and from airflow. Furthermore, the site is near a cliff, and many trees are nearby. One possible way to model such a situation is to assume that each source of eddies has a von Karman spectrum with an outer scale the size of that source. Then the total from all such sources (each with its relative strength) may lead to a spectrum that is shallower than the Kolmogorov spectrum. However, this model would be conjectural and would not be possible without complete measurements to ascribe strengths and sizes to each possible source. Also, if the Taylor hypothesis of frozen flow does not apply, the description of the phenomena becomes even more difficult.

If we consider all of the possible sources of near-ground turbulence in the SSL experiment, it may not be unreasonable to assume a random walk spectrum for the very lowest layer of the atmosphere, as the SSL group has speculated. The multiple-phase-screen code allows such a spectrum to be used on a screen close to the observation point, and the upper screens can be set with a Kolmogorov spectrum. By adjusting the propagation path length for the screen, the strength of the fluctuations, and the power law for the phase spectrum used to create the screen, we can observe the effects on optical observations of a non-Kolmogorov power spectrum near the ground. We are continuing efforts along this line.

The usefulness of the phase-screen approach for modeling non-Kolmogorov regions of the atmosphere will be further demonstrated when information from Russian investigators is available. Gurvich and other Russian investigators found layering in the upper atmosphere, which causes scintillation effects at visible wavelengths over long propagation paths.⁹ This layering is believed to have a spectrum associated with stratospheric internal waves and hence would not be Kolmogorov. The possible effects of this layering on sodium laser guide stars is an issue that can be addressed with our code.

As a measure of the strength of medium fluctuations, we use the parameter U (Ref. 10). When U is below 0.3, the weak fluctuation regime is applicable, and most fluctuation effects can be calculated analytically. For example, the intensity variance in this regime would be exactly equal to U . However, certain effects, even in the weak-fluctuation regime, cannot be easily calculated analytically. For example, the high-wave-number tail of the intensity spectrum is not well predicted by weak-fluctuation theory. Other effects of the high-wave-number tail may be important to adaptive optics; i.e., the rapidity with which the adaptive-optics system must respond (the bandwidth) may be controlled by this tail. Therefore, our numerical simulation technique is particularly useful: First, it is easier to apply than possibly complicated numerical integrations from analytical formulas; second, it is more general because effects outside the weak-fluctuation approximation are automatically simulated.

The real atmosphere appears to be composed of numerous thin layers, with significant differences in C^2_n from one layer to another. When there are relatively strong layers at high altitude, moving with high velocity, rapid scintillation from small-scale structure can adversely affect systems that cannot compensate rapidly enough. Thus, the SSL experiment is limited by the ability of the system to track fringes in the infrared because variations in phase can exceed 2π over very short times. The use of multiple phase screens allows intensity and phase effects to be properly modeled together.

This was demonstrated by a comparison of results obtained from using the multiple-phase-screen code with two model atmospheres. The first is the so-called Hufnagel Valley 5/7 model, with an upper atmospheric wind of 21 m/s (Ref. 11). This model leads to a calculated value of the Fried coherence length, r_0 , of 5 cm, an isoplanatic angle of 7 mrad (about 1.4 arcsec), and a U of 0.08. The value of r_0 indicates, by astronomical standards, relatively poor seeing.

The second model is relevant to the Mauna Kea site and is taken from a report by an LLNL group.¹² This model gave an r_0 of 15 cm (good seeing), an isoplanatic angle of about 3.1 arcsec, and a U of 0.04. The ratios of quantities between the two models are different for different quantities. The r_0 at Mauna Kea is three times larger (better) than for the Hufnagel model, but the root-mean-square amplitude fluctuations are only 1.4 times smaller (better). Thus, the quality of seeing may not scale easily with the measured scintillation, in agreement with measurements by Sarazin at sites in Chile.¹³ Our work on these topics is continuing.

1. Bester, M., W. C. Danchi, C. G. Degiacomi, L. J. Greenhill, and C. H. Townes (1992), "Atmospheric Fluctuations—Empirical Structure Functions and Projected Performance of Future Instruments," *Astrophys. J.* **392**, 357.
2. Bely, P.-Y. (1987), "Weather and Seeing on Mauna Kea," *Publ. Astron. Soc. Pac.* **99**, 560.
3. Walters, D. L., V. J. Gast, T. S. Mattingly, and D. Galarowicz, (1992), "Atmospheric Characterization for the Air Force—Maui 4-m Telescope," in *Technical Digest for the Adaptive Optics for Large Telescopes Topical Meeting* (Optical Society of America, Washington, DC), p. 51.
4. Salmon, D. (1992), "Mirror, Dome, and Local Seeing Effects at the CFHT," in *Technical Digest for the Adaptive Optics for Large Telescopes Topical Meeting* (Optical Society of America, Washington, DC), p. 17.
5. Vernin, J. (1992), "Atmospheric Turbulence Profiles," presented at the Scintillation Conf. (University of Washington, Seattle).
6. Armstrong, J. W., and R. A. Sramek (1982), "Observations of Tropospheric Phase Scintillations at 5 GHz on Vertical Paths," *Radio Science* **17**, 1579.

References

7. Shannon, R. R., W. S. Smith, W. Metheny, C. Ceccon, and R. Philbrick (1979), "New Experimental Data on Atmospheric Propagation," *Science* **206**, 1267.
8. Nightengale, N. S., and D. F. Buscher (1991), "Interferometric Measurements at La Palma," *Mon. Not. R. Astron. Soc.* **251**, 155.
9. Grechko, G. M., and A. S. Gurvich (1990), "Thin Stratified Structure of the Middle Atmosphere," *Adv. Space Res.* **10**, 21.
10. Martin, J. M., and S. M. Flatte (1988), "Intensity Images and Statistics from Numerical Simulation of Wave Propagation in 3-D Random Media," *Appl. Opt.* **27**, 2111.
11. Sasiela, R. J. (1988), *A Unified Approach to Electromagnetic Wave Propagation in Turbulence and the Evaluation of Multiparameter Integrals*, Massachusetts Institute of Technology Lincoln Laboratory, Lexington, MA, Technical Report 807.
12. Olivier, S. S., C. E. Max, D. T. Gavel, and J. M. Brase (1992), *Resolution Limits for Ground-Based Astronomical Imaging Using Adaptive Optics*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-109219.
13. Sarazin, M. (1992), "The Use of the Large Spatial Coherence of Turbulence Patterns for Predicting Observing Conditions in Astronomical Observatories," presented at the Scintillation Conf. (University of Washington, Seattle).

Observations with the Berkeley-IGPP Mid-Infrared Array Camera

Principal Investigator: Jack Welch (UC Berkeley)

LLNL Collaborator: Christopher J. Skinner

Other Collaborator: Eric Arens (Space Sciences Laboratory, UC Berkeley)

Student: Margaret Meixner (UC Berkeley)

The existence of bipolar planetary nebulae suggests that the mass loss, which drives an asymptotic giant branch (AGB) star to become a planetary nebula (PN), assumes a bipolar morphology before reaching the PN stage. Using the Berkeley mid-infrared camera, we are tracing the evolution of the circumstellar envelope (CSE) created by mass loss with images of AGB stars, PN, and protoplanetary nebulae, to determine at which stage the CSE changes shape.

Abstract

The last stages of stellar evolution in low- and intermediate-mass stars are critically affected by extreme mass loss on the asymptotic giant branch (AGB), which creates a dense and dusty circumstellar envelope (CSE). It has been suggested that CSEs assume a bipolar morphology as a consequence of the mass loss in about half of the evolved stars before reaching the planetary nebula (PN) phase. Our goal was to determine whether the morphology of the CSE changes with evolutionary phase and if so, at which phase. Using the mid-infrared (8- to 13- μ m) array camera at the UC Berkeley-IGPP Laboratory for Experimental Astrophysics, we imaged, at high angular resolution (<1 arcsec), a large sample of AGB stars, planetary nebulae (PNe), and protoplanetary nebulae (PPNe), which are objects in transition.

Objectives

Using the Berkeley mid-infrared (10- and 20- μ m) array camera at the United Kingdom Infrared Telescope and the Infrared Telescope Facility on Mauna Kea, we collected a large sample (~40) of AGB stars, PPNe, and PNe at less than 1-arcsec resolution. We resolved the CSEs of several AGB stars, enabling us to determine the size of the dust shells. In two M supergiants, α Orionis and μ Cephei, we found interesting nonspherical extensions to the dust shells. The structures in these high-mass analogs to the AGB stars could be explained either by a nonspherical mass-loss process or a nonspherical illumination of the dust shell.¹ In the latter scenario, the appearance of the dust shell should change over short timescales (months) because of the rotation of the star; hence, we are monitoring the shape of the mid-infrared emission in α Orionis and μ Cephei.

Progress

The PPN stage is the short-lived (less than a few hundred years) transition phase of the star as it evolves from the AGB to the PN stage. In fact, changes in these objects have been reported on timescales of decades (e.g., CRL 618). In recent years, searches for PPNe have revealed dozens of new candidates, characterized by Infrared Astronomy Satellite (IRAS) emissions, that peak at 10 and 20 μ m (indicative of a detached dust shell) and in some cases, optically visible central stars, e.g., high-latitude F and G supergiants. In the mid-infrared, we imaged the structure of the detached dust shell in several PPNe and found elongated and bipolar morphology in mostly carbon-rich PPNe and spherically symmetric shapes in mostly oxygen-rich PPNe (Figure 1). This correlation of chemistry with morphology suggests that bipolar PNe evolve from carbon stars.

Our images of young PNe, which have spectral energy distributions peaking near $20\ \mu\text{m}$, provide insight into the final shaping of PNe by the ionization front. We studied in detail the structure of one young PN, IRAS 21282+5050, and found an elliptical torus of dust emission similar to that in NGC 7027 (Ref. 2). Furthermore, our mid-infrared images have similar resolution to radio continuum maps from the Very Large Array radio telescope, and comparison of the two wavelengths reveals the relative distributions of dust and ionized gas in a PN. Contrary to what is expected, we found that the dust and gas are not always coextensive; sometimes the dust extends further than ionized gas, and sometimes the ionized gas extends further than the dust.³ Finally, we are investigating the nature of polycyclic aromatic hydrocarbons (PAHs), which emit discrete features in the $10\text{-}\mu\text{m}$ window (7.7 , 8.2 , and $11.3\ \mu\text{m}$). Discovered first in the PN of NGC 7027, PAHs are thought to be a significant constituent of carbonaceous interstellar dust. In the simple geometry of a PN, any differences in the excitation of the features would appear as differences in their respective radial distributions. We are studying the spatial distributions of the PAH features in several PN.

Figure 1. Mid-infrared images of the structure of the detached dust shell in two PPNe. (a) Mostly carbon-rich PPNe have elongated and bipolar morphology, whereas (b) mostly oxygen-rich PPNe have spherically symmetric shapes.

References

1. Skinner, C. J., M. Meixner, G. Hawkins, J. G. Jernigan, and J. F. Arens (in press), "Mid-Infrared Images of Asymptotic Giant Branch Stars," *Proc. IAU Colloq.* **155**.
2. Ball, R., J. F. Arens, J. G. Jernigan, E. Keto, and M. Meixner (1992), "Thermal Dust Imaging: The Onset of Asymmetry in the Ultracompact HII Region G5.89-0.39," *Astrophys. J.* **389**, 616.
3. Meixner, M., C. J. Skinner, J. R. Ball, J. G. Jernigan, and J. F. Arens (in press), "Mid-Infrared Images of Planetary Nebulae," *Proc. IAU Colloq.* **155**.

Geosciences

Analysis of Weak and Strong Ground Motion Recordings of the Loma Prieta Earthquake and Aftershocks

Principal Investigator: Ralph Archuleta (UC Santa Barbara)

LLNL Collaborator: Steve Jarpe

Student: Grant Lindley (UC Santa Barbara)

We have studied recordings of the October 1989 earthquake near Loma Prieta, California, and its aftershocks to look for evidence on nonlinearity in site response and to study source scaling of earthquakes. We calculated nonlinear least-squares fits to the Fourier amplitude spectra for both the main shock and the aftershocks. We found no clear evidence for a widespread nonlinear site response. The scaling of the earthquake source indicates a possible breakdown of similarity between the main shock and its aftershocks: The source spectral falloff that best fits the data has a frequency ω significantly greater than ω^{-2} .

Abstract

The objectives of this study were to search for nonlinearity in site response and to study the source scaling of earthquakes using spectra from the October 1989, Loma Prieta, California, earthquake, which had a magnitude of 7.1, and its aftershocks. To accomplish these objectives, we fitted the Fourier amplitude spectra of the earthquake to a model for the earthquake source. We determined the attenuation in the spectral fits by using the parameter t^* , which is the travel time divided by the quality factor of attenuation Q . (Some researchers call this parameter k .) The parameter t^* can be determined at each site for the main shock and the aftershocks. An increase of t^* for the main shock compared to aftershocks would indicate nonlinearity.

Objectives

To test the scaling of earthquakes with source size, we divided the spectra of the main shock by the spectra of the aftershocks. Since the site and path effects should be similar for the main shock and the aftershocks, the division of the spectra leaves only the ratio of the source spectrum of the main shock to that of the aftershocks. Then we can calculate nonlinear least-squares fits to the spectral ratios to determine source parameters such as the source spectral falloff and the corner frequencies of the aftershocks.

To determine the attenuation parameter t^* , we fitted the spectra of the Loma Prieta main shock and aftershocks recorded at 15 sites. When we compared t^* between the main shock and the aftershocks at soil and rock sites, we found that t^* was clearly larger on average soil sites. This difference is explained by linear attenuation in the near surface, which is greater at soil sites. If attenuation were nonlinear, the t^* values for the main shock would be greater than the t^* for the aftershocks at soil sites. We observed no significant differences, which indicates that nonlinear site effects are not widespread in the data set.

Progress

To study the source scaling of earthquakes, we divided the Fourier spectra of the Loma Prieta main shock by the spectra of its aftershocks at sites that recorded both the main shock and aftershocks. Then we calculated nonlinear least-squares fits to the spectral ratios. One of the important parameters in the fits is the source spectral falloff—the rate at which the source spectra intensity drops at high frequencies above the spectral corner frequency. A source spectral falloff of ω^{-2} is generally considered consistent with earthquakes possessing a self-similar source scaling. The best fit to source spectral falloff at most of the sites that we studied is closer to ω^{-3} (Figure 1). These results suggest that there is a fundamental breakdown in similarity between the Loma Prieta main shock and its aftershocks.

Figure 1. Source spectral falloff for the October 1989 earthquake near Loma Prieta, California, and its aftershocks. The best fit to the source spectral falloff at most of the sites we studied is closer to ω^{-3} instead of ω^{-2} , which indicates a fundamental breakdown in similarity between the Loma Prieta main shock and its aftershocks.

Imaging the Magma Chamber at Long Valley Caldera Using Teleseismic Tomography with Three-Dimensional, Minimum Travel-Time Ray Tracing

Principal Investigator: Lee Steck (U.S. Geological Survey and UC Santa Barbara)

LLNL Collaborator: Jay Zucca

Student: Charles Weiland (UC Santa Barbara)

Abstract

We incorporated a three-dimensional minimum travel-time ray tracer into a teleseismic tomography algorithm. The ray tracer is robust, particularly in the presence of low-velocity bodies, which cause the seismic wave to diffract around the body. The ray tracer thus provides more accurate information about the ray path, which in turn can be used to better estimate the velocity structure sampled by the ray paths. To address the nonlinearity introduced by ray bending, we used an iterative approach to solve the tomographic inverse problem. Preliminary results show that a 250-km³ body with a 20% slower velocity is located directly beneath the resurgent dome of Long Valley Caldera between 4 and 14 km below the surface.

We implemented the simulated annealing algorithm to invert teleseismic polarization data from the Long Valley Caldera. Data come from three deployments of UC Santa Barbara and LLNL instruments. Results from synthetic tests show simulated annealing can be successfully used to invert polarization data. The synthetic data were generated from an asymmetrical low-velocity zone having a 30% perturbation from background. For seven stations and eight earthquakes, the inversion recovers 50 to 70% of the input velocity perturbation. However, the inversion residuals for this test are larger than the accuracy of the standard measurement techniques, suggesting that further tuning of the algorithm could produce even better results. We are working toward solving this problem and inverting the real Long Valley data.

Objectives

Several geophysical studies suggest that the Long Valley Caldera region of California overlies a sizable magma chamber. However, the shape and the velocity contrast of this zone are widely debated. A traditional technique used to image such a body is seismic tomography. However, the low seismic velocity associated with magma or partially molten bodies may cause a seismic wave to diffract around them. The one- and two-dimensional ray tracers traditionally used in seismic tomography cannot accurately locate diffracted ray paths; their use can lead to errors in computing the arrival time. By incorporating a minimum-time, three-dimensional ray tracer into a teleseismic tomography code, we hope to more accurately define the shape and magnitude of the low-velocity body.

In a previous study, we found that the polarizations of teleseismic P waves recorded at the Long Valley Caldera were highly anomalous and that a heterogeneous velocity structure under the caldera was causing these perturbations.¹ Our objective was to develop a method of inverting these polarization data. We chose the simulated annealing inversion algorithm because it can handle highly nonlinear problems and it can be implemented with ease.

Progress

In FY 1992, we completed the computer code that performs the three-dimensional ray tracing and the tomographic velocity model estimation. Extensive tests using synthetic velocity anomalies indicate that three-dimensional ray tracing does in fact lead to more accurate images of regions with large-magnitude, anomalously slow bodies.

We obtained preliminary results from the Long Valley region using data provided by Phil Dawson and coworkers of the U.S. Geological Survey (USGS).² The velocity structure was parameterized into six layers between 9.5 and 10.5 km thick with nodes evenly spaced on a 5-km grid. The background layer velocities are from Dawson et al. To account for the shallow structure, we used the station corrections to the arrival times that Dawson et al. computed from forward modeling.

Our results show that a sizable body with a large (20% or greater) velocity anomaly is centered beneath the resurgent dome of Long Valley Caldera extending from approximately 5 to 15 km below the surface. The size of the low-velocity body is similar to that found by Dawson et al., but the amplitude for the velocity anomaly that we found is much larger. The presence of velocity anomalies in the first layer throughout the caldera region may indicate that delays due to surface sediment structures are not yet modeled properly. Better modeling of the surface to depths of 6 km should not change the shape but could affect the amplitude of the large perturbations that we found beneath the resurgent dome. Improved modeling will also allow us to better image the lower-crustal and upper-mantle region, which shows a significant region of relative high velocity beneath the resurgent dome.

The simulated annealing inversion code has been written, and we tested it on both synthetic and real data. We implemented the program on an IBM RS-5000 computer. The simulated annealing algorithm that we chose was an offshoot of the Freeze Bath method of Basu and Frazer.³ First, we identified the so-called freezing temperature through a series of constant temperature runs. Then to invert the data, we performed slow cooling runs beginning just above the freezing point. The synthetic velocity model used to test the program was parameterized with a $9 \times 9 \times 7$ grid, where the continuous velocity zone was placed in layers 4 and 5 (at 8- and 12-km depth, respectively). In layer 4, the zone was nearly square and covered a 12×12 -km area. In layer 5, the zone was L-shaped, with dimensions of 12×20 km, and was slightly offset from the shallower portion. The background velocity consisted of a typical vertical gradient. We traced rays to seven stations and measured polarization perturbations at these stations from eight synthetic teleseisms. In the inversion, only velocities in layers 4 and 5 are unknown parameters. Velocities above and below this zone were fixed.

Each inversion used a different random number string and tested 1000 random models. About 60 hours of central processing units (CPUs) were required. The final stacked model achieved 87% reduction in variance from the input model (which consisted of a series of vertical gradients with no lateral variations). The shallower (1-km) layer is better resolved than the deeper (12-km) layer. At 1 km, the model recovers about 66% of the low-velocity anomaly, although it covers an area that is just slightly smaller than the true one. At 12 km, the model recovers about 50% of the velocity perturbation over an area about 70% smaller than the true one. To determine which nodes affect the results most, we generated maps of the variance of the velocity node values over the 17 simulated annealing runs. Those nodes with low variance are generally well resolved and are important in producing ray perturbations at the test stations.

The misfits between polarizations determined from the final and input models can be as large as 8 km/s in apparent velocity and 50 deg in bearing. These misfits are unacceptably large, since array measurements are typically accurate to 10 deg in bearing and 2 km/s in apparent phase velocity. Presumably, our fits would improve

as we sampled more of the model space, but such sampling could use exorbitant amounts of CPU. However, part of the problem lies in how we sample the model space. By adding completely random perturbations to the velocity model, we selectively search a subset of model space that contains very rough models. Since the anomalies we are searching for are smooth, the algorithm has a difficult time finding the correct solution. Therefore, to improve the performance of our algorithm, we must include some prior smoothing of the random models.

We also performed preliminary studies to invert the Long Valley Caldera data. In these tests, we inverted for velocity in the entire crust. We found that the problem was poorly constrained and that random models with no spatial correlation fit the data with about a 66% reduction in variance. Tests performed by adding random noise of varying standard deviation to the correct model showed that the error function had an extremely narrow minimum at the correct model. Thus, very small amounts of random noise would create significant errors in polarization. Again, part of the problem lies in how we create random perturbations to the model. By incorporating smoothing and constraining upper crustal shallow velocity structure using results from local earthquake tomography, we believe that the Long Valley data can be successfully inverted for deeper crustal velocity structure.

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1. Steck, L. (1991), *Array Analysis of 3-Component Teleseismic P and P-Coda Waves for Crustal Structure at Long Valley Caldera, California*, Ph.D. thesis, University of California at Santa Barbara.
 2. Dawson, P. B., J. R. Evans, and H. M. Iyer (1990), "Teleseismic Tomography of the Compressional Wave Velocity Structure beneath the Long Valley Region, California," *J. Geophys. Res.* **95**, 11021.
 3. Basu, A., and L. N. Frazer (1990), "Rapid Determination of the Critical Temperature in Simulated Annealing Inversion," *Science* **249**, 1409.

References

Inferring Earth Rheology from GPS Data

Principal Investigator: Duncan Carr Agnew (UC San Diego)

LLNL Collaborator: John Rundle

Student: Hadley O. Johnson (UC San Diego)

Abstract

We have investigated how to design geodetic networks and conduct global positioning system surveys to best estimate parameters that occur in simple earthquake-fault models. For a strike-slip fault, we found that with a typical series of measurements, we can estimate the slip rate and locking depth with a standard deviation of 25 and 30%, respectively.

Objectives

Crustal deformation research has increased in the last few years mainly because inexpensive, highly accurate global positioning system (GPS) equipment has become available. With this equipment, many new geodetic studies have become feasible. One interesting study, to which our work is a prelude, would be an attempt to measure the viscosity of the asthenosphere of the Earth. At present, the only technique available is to monitor the rate of postglacial rebound. Work in this area has provided valuable information, but the estimates of Earth rheology vary widely. We believe that by monitoring the time-varying deformation after a large thrust-zone earthquake using geodetic techniques, we should be able to add independent estimates of the Earth's viscosity to this continuing debate. Some of the questions we want to investigate include where to make the geodetic measurements, how often to repeat the measurements, and what accuracy we could expect for estimates of the rheological parameters.

Progress

We have made substantial progress on the strike-slip faulting study, which is a necessary step before we can begin the more complicated thrust-zone case. The overall strategy used in our programs is to simulate geodetic data on the computer using a model of earthquake faulting and a model of the expected stability of the geodetic monuments used to make the measurements. We invert this synthetic data set to estimate the parameters in the fault model. We repeat the entire process using a different realization of the noise sources in the error models and make another estimate of the parameters. When we have created and inverted a statistically large sample of data sets, we calculate the average values and confidence intervals for the fault-model parameters.

The strike-slip fault model that we investigated is the "standard" model of dislocation theory of an infinitely long, straight fault embedded in a purely elastic half-space. The top H meters of the fault are considered to be locked in place, and the lower section (to infinite depth) is assumed to slip freely at S m/y as a result of tectonic stresses. This model results in a deformation field that depends only on the distance from the fault trace, x , through the equation $\Delta(x) = (-S/\pi)\tan^{-1}(x/H)$.

For a typical measurement series where the position of 20 geodetic stations is monitored each year for six years, our results show that the two fault-model parameters, slip rate and locking depth, can be estimated with a standard deviation of approximately 25 and 30%, respectively, of their expected values. If stations are

monitored for 10 years, the standard deviations drop to about 17 and 21%. However, to obtain this same accuracy in a six-year period, we would need nearly 100 stations in the network.

Our results also show that significant gains can be made in small networks by locating stations in their optimal positions. As the number of stations is increased, this advantage decreases; thus, by the time a network includes more than about 20 stations, we gain little by optimizing the locations.

Since the basis of our study is in simulations, we needed an optimization technique that could deal with probabilistic functions. The method of simulated annealing fits this requirement and has worked well. Figure 1 graphically depicts the annealing process for a network of five stations located within four locking depths of the fault trace. At the top of the figure, the stations are positioned randomly. As the optimization proceeds (toward the bottom of the figure), the stations slowly move to their optimal locations. By carefully monitoring the progress of the optimization, we can also learn a great deal about why the geodetic stations are placed where they are and thereby understand how the fault model and error models interact.

Figure 1. Optimization of GPS observing station locations along a strike-slip fault using a simulated annealing algorithm. In the simulation, as the annealing temperature decreases (ordinate), the station locations (abscissa) “freeze” into their optimal configurations, i.e., the optimal distances normal to the strike-slip fault.

The Inversion of Surface-Wave Phase-Velocity Measurements for Lithospheric Structure beneath the Western United States

Principal Investigator: Charles J. Ammon (UC Santa Cruz)

LLNL Collaborator: Howard Patton

Abstract

We have inverted an expanded seismic surface-wave phase-velocity data set to determine lateral variations in phase velocity beneath the western United States. The data coverage is good for Love and Rayleigh waves with periods between 10 and 40 s. For the nonlinear tomographic inversion, we incorporate geologic smoothness constraints and show that the data are for the most part consistent with a correlation in velocity within tectonic provinces. The Sierra Nevada have slow phase velocities, indicative of a crustal root beneath this mountain range. Within the largest tectonic province sampled, the Basin and Range, the data require lateral variations in shear velocity between the northwest, northeast, and central regions.

Objectives

Using phase-delay measurements of Rayleigh and Love waves for approximately 50 western U.S. earthquakes, we estimated the lateral phase-velocity structure of the region to a resolution on the order of 100 km. Surface-wave phase-velocity maps are useful for investigating first-order geologic variations throughout the western United States and for direct application in near-real-time modeling of moderate-size earthquakes that occur within the region.

Progress

We have expanded a seismic surface-wave phase-velocity data set and estimated the lateral variations in phase velocity beneath the western United States. The expanded data contain more than double the previously available Love-wave measurements. In all, we processed about 100 Rayleigh- and Love-wave paths and incorporated them into a nonlinear tomographic inversion for the lateral variations in phase velocity between 10 and 40 s.

We modified the inversion technique to incorporate geologic smoothness constraints. This approach is a compromise between an unconstrained inversion and a rigid regionalized inversion approach. Velocities within each tectonic province must correlate over a specified distance (a few hundred kilometers), but velocities across tectonic boundaries are uncorrelated. With this a priori information incorporated in the inversion, the resulting model contains heterogeneities across tectonic boundaries that are directly constrained by the observations and not simply a result of inadequate or anisotropic data coverage.

The resulting models show that the largest velocity heterogeneity lies along the coast, particularly in California (Figure 1). Dramatic ray-bending effects are visible for waves traveling down the length of California, thus illustrating the necessity for the nonlinear tomographic analysis. The identification of regions prone to strong ray bending is important for analyzing seismic sources because the azimuth of the surface wave can vary by up to 20 deg from the azimuth predicted using the great-circle path.

Preliminary interpretations of the phase velocities in terms of geology have identified some areas for more detailed study. Across California, the thin crust beneath the Coast Ranges results in a strong phase-velocity gradient between the coast and the Central Valley, a region of relatively slow velocities, particularly at the shorter periods (10 to 20 s). Slow phase velocities indicate that the crust is relatively thick beneath the Sierra Nevada, consistent with the existence of a root beneath this mountain range. The structure beneath the Basin and Range can be separated into three regions: the northwest, northeast, and central. In the northwest, the phase-velocity variations suggest that the crustal structure is relatively fast in the lower crust and upper mantle. In the northeast, the upper crust is relatively fast, the crust is most likely thin, and the upper mantle is slow relative to the northwest Basin and Range. In the central Basin and Range, including the region surrounding Death Valley, the velocities are slightly slower. The Colorado Plateau has relatively small phase-velocity anomalies, an unusual observation since the crust beneath this region may be up to 50 km thick.

Figure 1. Surface-wave tomography results for the western United States. This map shows the lateral phase-velocity variations for 20-s Rayleigh waves. The inversion incorporates a priori constraints defined by the geologic province boundaries.

Receiver Function Modeling for Homogeneous Crustal Structure and Moho Topography: The Use of Other Body-Wave Constraints

Principal Investigator: Jean B. Minster (UC San Diego)

LLNL Collaborator: George Zandt

Student: G. Eli Baker (UC San Diego)

Abstract

We applied various constraints to reduce the inherent ambiguities of receiver function interpretation in modeling the crustal structure beneath the very broad-band seismic station at the Piñon Flat Observatory, California. We used surface P and S velocities from a borehole and midcrustal P and S velocities from a local travel-time tomography study to constrain depths to discontinuities inferred from the receiver function waveform modeling. We also tested inferences of Moho topography from azimuthal variation of travel times and amplitudes of the receiver Ps phase using various independent seismic data.

Objectives

There are many ambiguities in the interpretation of receiver functions, even for laterally homogeneous structures. One of the most basic is the tradeoff between depth to a discontinuity and an average velocity above the discontinuity. The inference of lateral velocity variations from single-station receiver functions is especially problematic. Azimuthal variations in timing and amplitude of arrivals may be caused by lateral velocity variations, topography of a discontinuity, or interference from reverberations from a slightly dipping, shallower discontinuity. Our objective is to try to resolve those ambiguities for a Piñon Flat Observatory (PFO) velocity model that was based initially on receiver functions, by adding as many additional constraints as we can determine.

Progress

Crustal modeling. We constructed forward models of the receiver function waveforms at PFO using constraints from other studies and other types of data to limit the acceptable models. By incorporating surface velocities obtained from a nearby borehole,¹ we placed the depth to a shallow velocity discontinuity more precisely at 3.4 km. Observation of P and S converted phases in the P waveforms of unprocessed seismograms from two regional underground nuclear explosions further confirms the existence of this discontinuity. By forcing our model to match the average slowness found in a local travel-time study,² we improved the constraints on the depths to discontinuities down the Moho. From the tomographic results, we also can assume that the low-velocity zone we modeled at 9-km depth is thin.

Moho topography. Azimuthal variations in the receiver function Moho Ps-P times (the Moho Ps is a converted seismic wave from the crust-mantle boundary) and Ps/P amplitude ratios indicate a deepening of the Moho to the northwest under PFO. Both sets of observations individually indicate some extent of nonplanar Moho structure. When taken together, they are strongly inconsistent with an explanation of the depth variation as entirely due to a planar-dipping Moho. To better understand the Moho topography, we stacked normalized vertical P-wave seismograms from events belonging to the same source region to enhance the PPmP phase. PPmP travel-time variations with azimuth also indicate a deeper Moho to the northwest, and the total variance is too great to be accounted for by a realistic planar-dipping structure.

Mislocation vectors³ calculated for the incident P waves indicate that rays are refracted by a major structure dipping to the southwest. Although this structure may be a major antiform 100 km below PFO,⁴ the lack of any signal from a steeply dipping Moho further suggests that depth variations may be caused by step offsets that separate areas of relatively horizontal Moho. Pn from a regional nuclear explosion was recorded across a temporary array deployed at PFO. Frequency–wave-number analysis and estimates of back azimuth and phase velocity from relative array arrival times give results consistent with a northwest-dipping Moho, although we again found indications of significant variations from a planar Moho.

Upper-mantle structure. A trough in the receiver functions immediately following the Moho Ps arrival at all azimuths, with azimuthal variation similar to the Moho Ps, is interpreted as the Ps phase from the base of a high-velocity mantle lid directly below the Moho.

We calculated velocity spectrum stacks (VSS) for receiver functions at PFO. With this technique, we can stack receiver functions from a broad range of ray perimeters by applying normal movement to each and thus enhance the upper-mantle converted phases. By plotting VSS over the same depth and velocity ranges, we further enhanced the VSS image and so more clearly imaged a discontinuity at 90-km depth (Figure 1). These arrivals are more distinct from the direction of the Gulf of California and are consistent with an explanation of the discontinuity as the base of the low-velocity zone of Walck's Gulf of California model, a feature that is not observed along the ray paths away from the Gulf.

Figure 1. The VSS for (a) Ps, (b) Pps, and (c) Ps and Pps phases for events with a southeast back azimuth. The many arrivals in the upper right of stack b are misstacked Ps arrivals. In stack c, only one major arrival remains, peaking at a depth of approximately 90 km and a stacking velocity of 3.8 km/s.

1. Fletcher, J., T. Fumal, H. Liu, and R. Porcella (1990), "Near-Surface Velocities and Attenuation at Two Boreholes near Anza, CA, from Logging Data," *Bull. Seis. Soc. Am.* **80**, 807.
2. Scott, J. (1992), *Microearthquake Studies in the Anza Seismic Gap*, Ph.D. thesis, University of California at San Diego.
3. Davies, D., and R. M. Shepard (1972), "Lateral Heterogeneities in the Earth's Mantle," *Nature* **239**, 318.
4. Walck, M. (1984), *Teleseismic Array Analysis of Upper-Mantle Compressional Velocity Structure*, Ph.D. thesis, California Institute of Technology, Pasadena.

References

Ion-Microprobe Analysis of Amino Acids in Meteorites

Principal Investigator: John F. Kerridge (UC Los Angeles)

LLNL Collaborator: Douglas Phinney

Abstract

We separated a suite of amino acids from the Murchison carbonaceous meteorite and analyzed them for the stable isotopes of carbon, hydrogen, and nitrogen. Data reduction is not yet finalized, pending completion of certain control experiments. Preliminary results reveal rather modest variations in isotopic composition between different amino acids, suggesting that their precursor compounds were derived from a fairly homogeneous presolar population.

Objectives

Despite general agreement that meteoritic amino acids were formed by chemical reactions occurring in the aqueous subsurface regions of asteroid-size parent bodies, the exact nature of those reactions and the source of the starting materials are still uncertain.¹⁻⁴ A key set of data potentially capable of addressing these questions consists of the compositions of the carbon, hydrogen, and nitrogen contained in those amino acids. Isotopic analysis of bulk amino-acid extracts has revealed significant enrichment in the heavier isotope for all three elements, ranging from 2.5% for ¹³C, 9% for ¹⁵N, and 175% for D, relative to standard terrestrial values.^{5,6} Of even greater significance, however, would be the distribution of the carbon, hydrogen, and nitrogen isotopes among individual amino acids. Previous studies of such individual isotopic compositions have shown broad qualitative similarity but marked quantitative disagreement.^{6,7} The objective of our study is to obtain accurate isotopic analyses of carbon, hydrogen, and nitrogen in a suite of individual amino acids separated from the Murchison carbonaceous meteorite.

Progress

Our approach to this problem focused on using the ion microprobe to generate the desired isotopic data. However, before we could perform an isotopic analysis, we had to separate the amino acids from each other and prepare each separated fraction for analysis. We explored alternative methods of separating the individual amino acids, namely vacuum sublimation and acid-column chromatography. Vacuum sublimation worked well for control samples but failed to achieve useful separation of naturally occurring mixtures of amino acids. We therefore used acid-column chromatography to generate different amino acid fractions, using high-pressure liquid chromatography (HPLC) to assay the amino acid content of each fraction.

We developed a procedure for preparing amino acid fractions for ion-microprobe analysis and refined our analytical technique so that it can yield carbon and nitrogen isotopic compositions with a precision, and probably an accuracy, of about 0.1%. Although this precision was adequate for our study, the amount of material required for analysis in the ion microprobe was comparable to that used in conventional stable-isotope analysis. The great potential advantage of the ion microprobe for small sample analysis was therefore not realized. In addition, we had persistent problems in achieving suitable precision for D/H measurement in the ion microprobe, and as a result, we decided to use the conventional analytical approach of sample combustion followed by gas purification and gas-source mass spectrometry.

Figure 1 shows our results for the column fractions containing the major meteoritic amino acids. Several features of these data should be noted. First, HPLC analysis revealed that amino acid separation was incomplete for most fractions. Because we know the proportions of the different acids in each fraction, we can still calculate the true isotopic composition of each amino acid. However, before we can make these calculations accurately, we must resolve a second problem revealed by the HPLC analysis—namely, that a non-amino acid component, apparently meteoritic but possibly including some column bleed, is also present in each fraction. To correct for the presence of that component, we must perform more control experiments, which we are developing.

A third problem can be recognized in the anomalously high nitrogen and hydrogen contents of the middle five fractions. This problem is clearly due to ammonia, which elutes from the acid column simultaneously with amino isobutyric acid. Again, correction for this interference is feasible but requires control experiments, which are ongoing. We have corrected the deuterium data for the contribution due to combustion blank but not for the exchange of readily exchangeable hydrogen in the amino acid carboxyl and amino groups. This correction also awaits the completion of the control experiments.

Finally, we must correct for a moderate level of terrestrial contamination that is apparent in the data for glycine and alanine. (Note that application of these corrections will result in a significant increase in the deuterium content of each fraction but will be particularly marked for those fractions toward that left side of Figure 1).

Although reduction of these data is not yet complete, it is already clear that they are potentially informative about the synthesis of the meteoritic amino acids and their precursor compounds. The fairly restricted ranges of isotopic values (when we allow for the likely effect of the corrections) indicate a fairly homogeneous population of

Figure 1. Abundances and isotopic compositions of carbon, nitrogen, and hydrogen in 14 amino acid fractions separated from the Murchison meteorite. Individual amino acids present in each fraction are identified as: GLY = glycine; ALA = alanine; AIB = amino isobutyric acid; ABA = amino butyric acid; and iVAL = isovaline. Note that the AIB-rich fractions are contaminated with ammonia, whose effect has not been corrected for.

precursor compounds, and the generally smooth variation of isotopic composition with fraction number suggests that at least the major amino acids in the Murchison meteorite were synthesized in a single episode. As noted elsewhere,^{2,4,5} the high deuterium contents suggest that the precursors were made in an interstellar molecular cloud and thus predated formation of the solar nebula.

References

1. Peltzer, E. T., J. L. Bada, G. Schlesinger, and S. L. Miller (1984), "The Chemical Conditions on the Parent Body of the Murchison Meteorite: Some Conclusions Based on Amino, Hydroxyl, and Dicarboxylic Acids," *Adv. Space Res.* **4**(12), 69.
2. Cronin, J. R., S. Pizzarello, and D. P. Cruikshank (1988), "Organic Matter in Carbonaceous Chondrites, Planetary Satellites, Asteroids, and Comets," in *Meteorites and the Early Solar System*, J. F. Kerridge and M. S. Matthews, Eds. (University of Arizona Press, Tucson, AZ), p. 819.
3. Shock, E., and M. D. Schulte (1990), "Amino-Acid Synthesis in Carbonaceous Meteorites by Aqueous Alteration of Polycyclic Aromatic Hydrocarbons," *Nature* **343**, 728.
4. Kerridge, J. F. (1991), "A Note on the Prebiotic Synthesis of Organic Acids in Carbonaceous Meteorite," *Origins of Life* **21**, 19.
5. Epstein, S., R. V. Krishnamurthy, J. R. Cronin, S. Pizzarello, and G. U. Yuen (1987), "Unusual Stable Isotope Ratios in Amino Acid and Carboxylic Acid Extracts from the Murchison Meteorite," *Nature* **326**, 477.
6. Pizzarello, S., R. V. Krishnamurthy, S. Epstein, and J. R. Cronin (1991), "Isotopic Analyses of Amino Acids from the Murchison Meteorite," *Geochim. Cosmochim. Acta* **55**, 505.
7. Engel, M. H., S. A. Macko, and J. A. Silfer (1990), "Carbon Isotope Composition of Individual Amino Acids in the Murchison Meteorite," *Nature* **348**, 47.

Constraints on the Origin of Oxygen Isotopic Anomalies in Meteorites

Principal Investigator: Kevin D. McKeegan (UC Los Angeles)

LLNL Collaborator: Frederick J. Ryerson

Using available diffusion data, we have calculated the rate of oxygen isotopic equilibration in a 1-cm molten sphere for various cooling rates representing the possible crystallization interval in calcium-aluminum-rich inclusions found in the Allende meteorite. The results indicate that the residual melt will be totally equilibrated for cooling rates of about 1°C/h. These rates are comparable to those inferred from textural studies and indicate relatively slow cooling rates for these objects. We are performing partial equilibration experiments on these materials to monitor the composition of the mineral phases during equilibration.

Abstract

Nucleosynthetic variations in oxygen isotopic compositions are ubiquitous among all meteorite groups and serve as a means of classifying planetary materials. Such variations also characterize whole rock samples of refractory calcium-aluminum-rich inclusions (CAIs) from the Allende meteorite and other carbonaceous chondrites, which define a single line on a diagram of $^{17}\text{O}/^{16}\text{O}$ vs $^{18}\text{O}/^{16}\text{O}$ with a slope close to unity. This Allende array can be described as a mixing line between a component of roughly solar/terrestrial composition and another component that is preferentially enriched in ^{16}O . Attempts to identify the carriers of the anomalous component revealed a systematic distribution in the relative concentration of the anomalous oxygen component among the minerals comprising CAIs.¹ The largest excesses of the ^{16}O -enriched component were found in spinels (about 4% excess) with clinopyroxene having somewhat lower concentrations.

Objectives

The compositions of melilite and anorthite lie much closer to the terrestrial composition. The patterns of isotopic anomalies observed in these meteoritic materials represent the convolution of (1) the initial isotopic composition imposed by some mixture of nucleosynthetic components emanating from various astrophysical settings, and (2) nebular and planetary processes. If the efficiency of the various processes responsible for such isotopic homogenization can be described as a function of external conditions, then we may be able to constrain the history and conditions of these nebular events and perhaps reconstruct the isotopic composition of the interstellar material prior to processing within the solar nebula. In this project, we are investigating the kinetics of oxygen diffusion in the minerals and melts that may affect oxygen isotopic equilibration in CAIs so we can assess these processes.

The systematic variation in ^{16}O excesses in different minerals suggests that crystal chemical control is important in whatever process is responsible for the Allende array. Diffusive exchange of oxygen between the various minerals in CAIs and a gas reservoir is one mechanism that could produce a consistent, systematic, and mineralogically controlled distribution of anomalous oxygen.² In this model, the initially uniform ^{16}O -enriched oxygen of the CAI undergoes partial isotopic exchange with more normal oxygen in the surrounding nebular gas. For the thermal history of any proposed solid-gas interaction, the time-integrated diffusivity of melilite and anorthite must exceed that of clinopyroxene, which in turn exceeds that of more refractory oxides such as spinel.

Progress

We have demonstrated that it is extremely difficult to produce the necessary fractionation by solid–gas exchange starting with an initially homogenous inclusion. Therefore, we have suggested that the pattern of anomalies has resulted from partial reequilibration of the inclusion while it was molten. For such a model to work, the composition of the melt during the final stage of crystallization would have to totally equilibrate with the terrestrial reservoir.

Using available diffusion data, we calculated the fractional equilibration f of a 1-cm, partially molten sphere for various cooling rates over the crystallization interval (Figure 1). The results indicate that the melt will be totally equilibrated ($f = 1$) for cooling rates of about $1^\circ\text{C}/\text{h}$. These rates are comparable to those inferred from textural studies and indicate relatively slow cooling rates for these objects. We are performing partial equilibration experiments on these materials to monitor the composition of the mineral phases during equilibration.

Figure 1.
Fractional isotopic equilibration f in a partially molten sphere 1 cm in diameter as a function of temperature for different cooling rates.

References

1. Clayton, R., L. Onuma, L. Grossman, and T. Mayeda (1977), "Distribution of the Pre-Solar Component in Allende and Other Carbonaceous Chondrites," *Earth Planet. Sci. Lett.* **34**, 209.
2. Clayton, R., and T. K. Mayeda (1977), "Correlated Oxygen and Magnesium Anomalies in Allende Inclusions I: Oxygen," *Geophys. Res. Lett.* **4**, 295.

Alteration of Mid-Ocean Ridge Basalt Glasses: Mobile Nuclides

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LLNL Collaborators: Marilyn ten Brink, Douglas Phinney, and Kevin Knauss

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We are measuring trace-element concentrations in a suite of natural glasses and in palagonite, the primary product of natural glass alteration, and are using the resultant data to improve our understanding of trace-element mobility during alteration reactions. This study is a natural experiment for the behavior of trace elements and radionuclides under geologically meaningful boundary conditions (low temperatures, open system behavior, long periods of exposure). It will provide data for understanding the mobility of trace elements during ocean-floor alteration and within an altered volcanic sequence and for determining the mass balance between ocean crust and seawater. Our results indicate that: (1) rare-earth elements (REEs) are affected by seafloor alteration on a large scale under only the most extreme alteration conditions, (2) trace-element abundances are heterogeneous in clay samples, and (3) REEs tend to follow the major elements during alteration of basaltic glass to palagonite.

Abstract

Silicate glasses and their alteration play an important role in industry and geology. High-level nuclear waste is fused into borosilicate glass and disposed of, using geologic repositories that contain large quantities of silicate glasses or their alteration products (e.g., at Hanford and Yucca Mountain). Silicate glasses are a common product of volcanism. They are the principal components of all explosive volcanoes and are common in all subaqueous volcanic environments, such as mid-ocean ridges and seamounts. Silicate glasses are chemically unstable; they readily hydrate and partly dissolve in water to produce various authigenic materials such as clays and zeolites, which remain geochemically active through ion exchange and sorption.

The net effect of these processes is that some elements are removed from circulating waters and others are mobilized. These exchange reactions are a topic of concern for understanding geochemical processes of global significance and for assuring environmental safety. Several trace elements are important in both respects, such as uranium, thorium, lead, strontium, and cesium. Substantive efforts have been expended in characterizing the alteration processes of synthetic and natural glasses under experimental conditions. This effort, however, has not been duplicated for trace elements in natural alteration conditions (low temperature, open system behavior, long periods of exposure). Little is known about the behavior of most trace elements during alteration of silicate glasses in such a geologic environment.

Our project is designed to address this issue. We are using various analytical techniques to study the chemical variation of natural glasses up to 120 million years old and their alteration products for a large suite of elements. We had two goals: (1) to analyze natural silicate glasses and their major alteration product, palagonite, for a suite of trace and major elements that are believed to be sensitive to alteration or are critical for studies of petrogenetic processes or paleoceanography or are important hazardous constituents of nuclear waste; and (2) to analyze some typical low-temperature authigenic phases separated from veins or vugs, to document potential hosts for elements that are liberated during silicate glass alteration. We

Objectives

want to study trace-element redistribution in the oceanic crust on the level of individual chemical reaction (in contrast to bulk-rock studies) and to provide important boundary constraints for the long-term chemical behavior of radionuclides in the geologic host environment.

Progress

In FY 1992, we collected samples in the field, finished inductively coupled plasma-mass spectrometry (ICP-MS) trace-element analysis of a suite of samples, completed mineralogical studies and sample characterization, and submitted a paper for publication. Our initial results indicated that rare-earth elements are affected by seafloor alteration on a large scale under only the most extreme alteration conditions. We found that (1) trace-element abundances are heterogeneous in clay samples, and (2) REEs tend to follow the major elements during alteration of basaltic glass to palagonite. Our work expands on these findings.

We used the clean sample digestion facility to process samples from drill holes made by the Deep Sea Drilling Project (DSDP) and from the Troodos Ophiolite. We solved the analytical difficulties with ICP-MS by moving to isotope dilution techniques and thus obtained satisfactory blank and calibration values.

We found that rare-earth elements are affected by seafloor alteration on a large scale under only the most extreme alteration conditions. We determined the REE bulk composition of mature oceanic crust for compositional domains in DSDP holes 417A, 417D, and 418A on length scales between 10 and 500 m. Compositional domains include two lithologic types, massive flows and volcanoclastic rocks, and provide a combined bulk estimate for the upper 500 m at these sites. Analysis of material from these DSDP holes showed that the bulk oceanic crust does not show significant change in REE patterns in the upper 500 m; however, the abundances can vary by up to 60% from fresh rock values in the most altered domains, because of passive accumulation and bulk dilution from additional REE-poor secondary phases. In hole 417A, we observed the seawater signature of light REE enrichment (up to 90% increase in lanthanum) with a negative cerium anomaly, which represents a seawater:rock ratio of $10^7:1$. The bulk crust shows enrichment of less than 3% (seawater:rock ratio $< 4 \times 10^5$), which is within the limits of analytical uncertainty. Much of the volatile and alkali inventory of the oceanic crust also resides in intensely altered zones, which may contribute disproportionately to metasomatic fluids and melts during subduction and crustal recycling and thus enhances the probability of extracting REEs that bear the signature of seafloor alteration.

We performed mineralogical studies on palagonite tuff from the island of Oahu and on glass, palagonite, and low-temperature secondary phases from the Troodos Ophiolite. We separated, characterized, and documented samples from a range of alteration conditions to prepare for analysis with the secondary ion mass spectrometer (SIMS). We located the samples that were large enough to allow SIMS transects across glass-palagonite-zeolite (not a simple task) since earlier work had indicated that transects across the boundaries provided more information than discrete analysis in each phase. Heterogeneity within the bulk material and within the alteration phases is sufficiently large that multiple analyses are required to obtain abundance values comparable to those obtained by dissolution and ICP-MS analysis of separates.

Incision by Rivers into Bedrock: A Test of Competing Erosion Mechanisms Using Cosmogenic Isotopes

Principal Investigator: William E. Dietrich (UC Berkeley)

LLNL Collaborators: Marc W. Caffee, Robert C. Finkel, and G. Bryant Hudson

Student: Michele A. Seidl (UC Berkeley)

We are analyzing the concentration of ^{26}Al , ^{10}Be , ^3He , and ^{21}Ne in rock samples collected along a river's longitudinal profile to determine the relative importance of two proposed incisional mechanisms: (1) vertical incision due to abrasion and dissolution and (2) stepwise lowering caused by knickpoint propagation, play in channel downcutting, and consequent profile development. The pattern of isotopic concentrations exhibited by the samples differs depending on which erosional mechanism is predominant.

Abstract

In FY 1992, we extensively studied a river that provides a testable and well-constrained framework in which to assess the isotopic results. We also calculated the long-term erosion rates. Preliminary isotopic, numerical, and field results suggest that knickpoints sweep upstream, leaving incised, steep-walled valleys in their wake, whereas channel lengths that are upstream of the knickpoints are eroded far more slowly by a suite of steady-state processes including abrasion and chemical weathering. Knickpoints may be linked to changes in boundary conditions during profile development, and knickpoint propagation may be of primary importance on all bedrock channels that develop under the conditions necessary to generate knickpoints.

River incision into bedrock is a key process linking landscape evolution with tectonics and climate change; yet no theory exists to predict how river longitudinal profiles develop in bedrock. There appear to be three processes by which bedrock channels erode: (1) vertical wearing of the channel bed due to stream flow, by such processes as abrasion by transported particles and dissolution; (2) scour by periodic debris flows; and (3) knickpoint propagation.¹ Surface-exposure age dating using cosmogenically produced isotopes allows us to quantitatively investigate the rates of incision by these processes.

Objectives

The main channel that we sampled is at depositional grade, which precludes debris-flow scour and led us to concentrate on differentiating between the relative importance of vertical wearing and knickpoint propagation. By simultaneously measuring both stable and radioactive isotopes in olivine separates, we can address the issue of surface burial by sediments.² Our goal is to understand how rivers carve into rock and to use this understanding to develop a general theory for river profile development into bedrock.

We completed the fieldwork and rock sampling in January 1992. To address the proposed mechanisms, we extensively sampled the olivine-rich rock in a single valley, Kaulaula Valley, Kauai. The principal channel of Kaulaula Valley has both bare bedrock and boulder-mantled reaches. The channel spills over a 50-m-high waterfall. We sampled the channel bed, boulder terraces, and valley walls of Kaulaula Valley. Most of the samples were collected using a sledge, but seven samples were collected by core drilling.

Progress

We separated olivines from 14 samples. We first analyzed samples for the noble gases ^3He and ^{21}Ne because these measurements do not necessitate dissolution and column chemistry. The results were interesting and consistent, except for one provocative analysis, which indicated that for more than 1 million years, a sample had retained its full complement of ^{21}Ne but had lost 90% of its ^3He .

Initial ^{10}Be measurements indicated the presence of meteoric ^{10}Be . Because we are interested in only the in situ-produced ^{10}Be , we performed several leaching experiments and measured the ^{10}Be content in each of the leachates to determine the most effective way to remove the meteoric material. Our results indicated that olivine grains must be washed in HF and HCl solutions prior to their dissolution. The chemistry involved in ^{10}Be and ^{26}Al sample preparation is complicated, so we wrote a protocol describing the steps. The bulk of previously published work detailing ^{10}Be and ^{26}Al results in rocks reported results from quartz aliquots, and only one reference reports ^{10}Be and ^{26}Al results from olivine separates.² Subsequent to finalizing the protocol, we analyzed four samples for ^{26}Al and two for ^{10}Be . In FY 1993, we will analyze 10 additional samples for the radioactive isotopes. Other samples are being crushed and separated prior to the chemical preparation.

Figure 1 shows our preliminary isotopic results. The data indicate that exposure ages decrease in the upstream direction from 1.5 million years to 0 years at the knickpoint and remain fairly constant above the knickpoint, which is consistent with knickpoint propagation. In contrast, abrasion and solution weathering are consistent with exposure ages increasing in the upstream direction. If we assume steady-state erosion, nuclides in the olivines will attain an equilibrium concentration $N(x,t)$, according to:

$$N(x,t) = \frac{e^{\mu x} P(0)}{\lambda + \mu \epsilon}, \quad (1)$$

where $\mu = \rho/\Lambda$ (ρ is the target density, and Λ is the absorption mean free path of the interacting particle), $P(0)$ is the nuclide production rate at the surface, λ is the decay constant, and ϵ is the erosion rate.³ Then the maximum age a sample can attain, T_{eff} , once equilibrium is reached, is $T_{\text{eff}} = N(0)/P(0)$.

If the average erosion rate above the knickpoint is 0.002 cm/y, then T_{eff} is approximately 35,000 years, which is the same order of magnitude as our measured exposure ages. If the average erosion rate below the knickpoint is 0.008 cm/y, then T_{eff} is approximately 7000 years, which is 2 to 3 orders of magnitude lower than our two oldest samples. These data, analyzed in concert with our understanding of long-term erosion rates, indicate a steady-state erosion above the knickpoint and decidedly nonsteady-state erosion below the knickpoint. These preliminary data are consistent with knickpoint migration and provide the first concrete evidence that large knickpoints may be extremely important in channel incision and drainage basin development. Clearly, the next 10 samples, which will fill in the data gap between the oldest boulders and the knickpoint, are of paramount importance to test the theory.

To further investigate how river profiles develop in Kauai, we performed numerical simulations assuming that sediment supply was not a constraint and that erosion rate was some function of stream power. The channels below the knickpoints on Kauai have slopes between 5 and 8 deg and are mostly straight. Such features cannot be produced by simple stream-power-based erosion theory, so some constraint must be limiting slope development. We propose that the boulder mantling of long channel reaches inhibits channel incision, thus reducing downcutting to a rate set both by knickpoint propagation sweeping under the boulder armor and by weathering of boulders. Partial boulder mantling of bedrock-dominated channels is common in mountainous regions, and a theory that considers boulder armoring will have broader application than one that ignores these effects.

Figure 1. Preliminary isotopic results from our study of the olivine-rich rock in the channel bed, boulder terraces, and valley walls of Kaulaula Valley, Kauai. The principal channel has both bare bedrock and boulder-mantled reaches, and it spills over a 50-m-high waterfall. The data are consistent with knickpoint propagation: In the upstream direction, exposure ages decrease from 1.5 million years to 0 years at the knickpoint; above the knickpoint, they remain fairly constant.

1. Seidl, M. A., and W. E. Dietrich (1992), "The Problem of Bedrock Channel Erosion," *Catena Suppl.* **25**, 133.
2. Nishiizumi, K., J. Klein, R. Middleton, and H. Craig (1990), "Cosmogenic ^{10}Be , ^{26}Al , and ^3He in Olivine from Maui Lavas," *Earth Planet. Sci. Lett.* **98**, 263.
3. Lal, D. (1991), "Cosmic Ray Labeling of Erosion Surfaces: In Situ Production Rates and Erosion Models," *Earth Planet. Sci. Lett.* **104**, 424.

References

Relation between Global Climate and the History of Desert Formation as Studied Using In Situ–Produced ^{10}Be , ^{26}Al , and ^{21}Ne in Quartz

Principal Investigators: Kunihiko Nishiizumi and James R. Arnold
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LLNL Collaborators: Robert C. Finkel, Marc W. Caffee, and G. Bryant Hudson

Abstract

We have measured ^{10}Be and ^{26}Al in sand and bedrock from several locations in Australia. The minimum ^{10}Be exposure ages of the sand are 300,000 to 800,000 years, a factor of 5 to 10 longer than the ages of sands collected from North America and Africa. The ^{10}Be concentrations decrease slightly with decreasing grain size. The minimum exposure ages of the bedrock measured here are similar to the ages of the sands. These ages correspond to erosion rates that are quite low, 1 m/million years or less. The similarity of the high ^{10}Be concentrations for both sands and bedrock illustrates the stability of landforms in the Australian continent.

Objectives

The surface of the Earth is continuously altered under the influence of weathering and erosion, plate tectonics, and volcanic processes. Continental denudation, which depends on complex rock–water interactions, is the central process of the global biogeochemical cycling of elements. Rates of denudation depend on several factors, in particular rock properties and chemical composition, climate (especially rainfall), and landform structure and elevation. A primary step in most geomorphologic studies is to better understand the location-specific weathering and erosional processes and their rates and cycles over different time periods. To determine the rates of these erosional processes, we applied a new technique that uses cosmogenic nuclides produced in situ in the surfaces of crustal materials.

Our study, a collaborative investigation to measure in situ–produced cosmogenic nuclides in terrestrial samples, especially sands, was performed at the UC San Diego Department of Chemistry and at LLNL's Nuclear Chemistry Division and Center for Accelerator Mass Spectrometry. Our goal is to study the history of desert formation during the past glacial cycle and earlier. In FY 1992, we measured the content of cosmic-ray–produced radionuclides (^{10}Be and ^{26}Al) and stable nuclides (^{21}Ne) in the same terrestrial quartz extracted from sands. We measured ^{10}Be and ^{26}Al using accelerator mass spectrometry, and we plan to measure ^{21}Ne using high-sensitivity noble gas mass spectrometry.

Progress

Cosmogenic nuclides have been applied to various problems in geomorphology, but they have not been applied to study desert sands. At present, cosmogenic nuclides may be the only quantitative measure of desert-sand formation and migration rates. The results obtained to date unambiguously demonstrate the potential of in situ cosmogenic nuclides to study processes of desert formation and evolution.

In FY 1992, we studied cosmogenic nuclides ^{10}Be and ^{26}Al in quartz extracted from a large number of terrestrial rocks and sands. Our goals were to measure the production rates of the nuclides and to use them as natural tracers for studying surficial processes such as erosion rates, apparent surface exposure ages, and surface exposure histories. As a part of this project, we made more than 40 ^{10}Be and ^{26}Al measurements in terrestrial quartz.

After studying a suite of sands from deserts throughout the world, we concentrated on measuring ^{10}Be and ^{26}Al in sand and bedrock from several locations in Australia. We also prepared grain-size separates from many of the sand samples so we could determine if grain size affects the dune-formation process. The minimum ^{10}Be ages of the Australian sand are 300,000 to 800,000 years—a factor of 5 to 10 longer than the ages of sands collected from other areas of the world. The minimum exposure ages of bedrock in various locations in Australia are long, similar to the ages of the sands. The maximum erosion rates of these rocks are quite low, 1 m/million years or less. The erosion rates alone, which are comparable to those obtained in low-erosion environments such as Antarctica, indicate that the bedrock formations on the Australian continent are stable structures.

The similarity of the high ^{10}Be and ^{26}Al concentrations for both sands and bedrock further illustrates the general stability of landforms on the Australian continent. Although the minimum exposure ages of bedrock and sand are similarly high, the sand has undergone a complex exposure history, unlike the bedrock (see Figure 1). Many of the bedrock points lie in the field of simple exposure, whereas the sand samples lie below this field, in a region indicating a complex history of exposure and burial.¹

We are measuring ^{21}Ne , so we can test this conclusion. Unlike ^{10}Be and ^{26}Al , ^{21}Ne concentrations yield the integrated exposure duration of a sample. As such, it is particularly useful when samples have undergone complex or multiple exposures. Grain-size distributions measured for the Australian sand samples show a large difference in the degree of sorting for various sand regions on that continent. The ^{10}Be concentrations and $^{26}\text{Al}/^{10}\text{Be}$ ratios decrease slightly with decreasing grain size for many samples. We are still trying to understand these results and attempting to relate them to models of sand production and transport in Australia.

Figure 1. Diagram of the concentration of $^{26}\text{Al}/^{10}\text{Be}$ and ^{10}Be for Australian sands and bedrock. The minimum exposure ages of bedrock fall within the steady-state erosion island; however, the sand data do not indicate its complex exposure history.

1. Nishiizumi, K., C. P. Kohl, J. R. Arnold, J. Klein, D. Fink, and R. Middleton (1991), "Cosmic-Ray-Produced ^{10}Be and ^{26}Al in Antarctic Rocks: Exposure and Erosion History," *Earth Planet. Sci. Lett.* **104**, 440.

References

Source Characterization of Atmospheric Carbon Monoxide in California by Radio- and Stable-Isotope Measurements

Principal Investigator: Isaac R. Kaplan (UC Los Angeles)

LLNL Collaborator: Jay C. Davis

Abstract

We have developed methods for collecting, isolating, and oxidizing 1 mg of atmospheric CO to analyze its isotopic ratios such as $^{14}\text{C}/^{12}\text{C}$ ($\Delta^{14}\text{C}$), $^{13}\text{C}/^{12}\text{C}$ ($\delta^{13}\text{C}$), and $^{18}\text{O}/^{16}\text{O}$ ($\delta^{18}\text{O}$). Using the ambient air collector that we developed, we can collect up to 600 L of ambient air into aluminum gas cylinders within about 30 min. The air collected in the cylinders was passed through the vacuum line, in which CO was purified, isolated, and further oxidized to produce CO_2 gas using Schutze reagent at room temperature.

We analyzed the CO_2 that emerged for carbon and oxygen isotopes using a stable isotope mass spectrometer ($\delta^{13}\text{C}$ and $\delta^{18}\text{O}$) at UC Los Angeles and an accelerator mass spectrometer ($\Delta^{14}\text{C}$) at LLNL. We tested the conversion efficiency of CO to CO_2 by a Schutze reagent, the blank level of CO in vacuum line, and the interference of atmospheric N_2O for measurements of the carbon and oxygen isotopes of CO. The results show that (1) the conversion of CO to CO_2 is quantitative, (2) a low level of line blank for CO is attained, and (3) no interference of N_2O for the CO measurements is observed. Therefore, the methods developed will be useful in measuring isotopes of atmospheric CO.

Objectives

Atmospheric CO, a toxic air pollutant, is a contributory gas to global warming and to the change of stratospheric and tropospheric ozone concentrations. Although the production mechanisms of CO in local air pollution are reasonably well known, the sources of background atmospheric CO are not well elucidated. In this study, we attempted to characterize sources of atmospheric CO by measuring its ^{14}C radioisotope ratio and its ^{13}C and ^{18}O stable-isotope ratios in various environments. These ratios are potentially important in differentiating modern carbon from fossil-fuel carbon and assigning source strengths to various biogenic sources, such as biomass burning and photochemical oxidation of biogenic hydrocarbons. We will estimate the contribution of contemporary carbon (modern carbon) for the source of atmospheric CO from the data of the ^{14}C measurement. Then we will identify the sources of contemporary carbon, such as methane and natural hydrocarbon oxidation and biomass burning, using measured $\delta^{13}\text{C}$ and $\delta^{18}\text{O}$ from CO.

This project will provide valuable information on the sources of atmospheric CO in southern California, which is among the largest emitters of CO in the mid-Northern Hemisphere. The information we will obtain will be helpful in estimating how industrial and agricultural activities contribute to local air pollution and to global climate change. Our objectives are to:

1. Develop the methodology for collecting, isolating, and oxidizing atmospheric CO to measure the isotopic ratios such as $\Delta^{14}\text{C}$, $\delta^{13}\text{C}$, and $\delta^{18}\text{O}$.
2. Identify the sources of CO in the atmosphere of southern California by determining the isotope ratios of $\Delta^{14}\text{C}$, $\delta^{13}\text{C}$, and $\delta^{18}\text{O}$ in CO.
3. Determine the diurnal and seasonal variations of isotopic composition of atmospheric CO to clarify the temporal variation of source strength of CO derived from various sources.

To measure the ^{14}C , ^{13}C , and ^{18}O contents of atmospheric CO , we must collect several hundred liters of air. For this task, we built an ambient air collector that can collect up to 600 L of ambient air within about 30 min using an oilless pump to minimize the contamination of hydrocarbons. We used aluminum gas cylinders (each with 13-L capacity) that can be pressurized up to 3300 psig, but we kept the pressure of the cylinders to 100 psig partly for safety reasons and partly because we do not have a pump that can work at higher pressures. The aluminum cylinders are more resistant to corrosion than the steel gas cylinders. A pressure switch shuts off the pump automatically when the pressure reaches the maximum 100 psig. Two air filters remove coarse and fine particles and more than 99% of water from the air. Both filters decrease the pumping efficiency and could contaminate the interiors of the gas cylinders. We pretested the air collector by pumping ambient air, and the results were satisfactory.

After we collect ambient air, we must isolate the CO and oxidize it to CO_2 gas for the isotope measurements. We developed an atmospheric CO purification, isolation, and oxidation system at the Isotope Laboratory at IGPP-UC Los Angeles (Figure 1). Ambient air collected in gas cylinders was introduced into a molecular-sieve column at a flow rate of 1 to 3 L/min to remove a large portion of water and N_2O . Next, the air was introduced into two liquid nitrogen traps to remove CO_2 , heavier hydrocarbons ($>\text{C}_3$), remaining water, and N_2O . After removing these gases, we used a Schutze reagent (I_2O_5) to convert CO gas to CO_2 gas at room temperature. Then the resultant CO_2 gas was collected in a cold finger, and the quantity

Figure 1. Vacuum line for purifying, collecting, and oxidizing atmospheric CO to CO_2 . The vacuum line is constructed with Pyrex and stainless-steel tubing and glass or Teflon stopcocks. The air sample was dried by an air filter and a molecular-sieve column during air collections.

was determined using a manometer. Finally, the CO₂ gas collected was sampled into a glass sample bulb and sealed. When we examined the conversion efficiency of CO to CO₂ by Schutze reagent, we found that CO is almost quantitatively ($99.4 \pm 2.7\%$) oxidized to CO₂. No other gases such as N₂O that are present in the ambient air seem to interfere or contaminate the oxidation of CO to CO₂. Thus, we believe the system is reliable for collecting and oxidizing atmospheric CO.

Using the ambient air collector and the CO isolation and oxidation system, we collected ambient air at Westwood in Los Angeles from July through September 1992 and measured the isotopes of atmospheric CO. The $\delta^{13}\text{C}_{\text{PDB}}$ of CO ranged from 25.2 to -26.9%, and we did not find a significant diurnal variation of the isotopic composition during the study period. Therefore, we suspect that CO derived from automobile emission is the major source of atmospheric CO at Westwood. However, wood burning, industrial product burning, and cooking might be other important sources of CO. We will investigate these possible sources in more detail during FY 1993, by measuring the carbon and oxygen isotopes.

Integrated Thermal, Hydrological, and Organic Geochemical Modeling of Sedimentary Basins

Principal Investigator: Chi-Yuen Wang (UC Berkeley)

LLNL Collaborator: Jerry Sweeney

Student: Eric Daymo (UC Berkeley)

Abstract

In FY 1992, we completed a finite-element program that couples thermal, hydrological, sedimentary, and organic geochemical processes in sedimentary basins. With this program, we can calculate methane and CO₂ generation and solubility in water, pore-pressure generation, and fluid transfer in an evolving basin. The results show that (1) the timing of methane and CO₂ are distinctly different, which leads to their distinct spatial distributions, and (2) methane and CO₂ production has little effect on pore pressures, so their production does not in itself drive the flow in the system.

Objectives

Below a depth of about 3000 m, fluid pressures exceed hydrostatic in more than half of the world's explored deep basins. Understanding the causes and characteristics of these fluid pressures is of major importance in exploring for and recovering hydrocarbon and mineral resources. Evidence accumulated during the past decade indicates that the generation of hydrocarbons and the compaction disequilibrium are probably the most important mechanisms in most sedimentary basins. Enough is understood about these processes that we can attempt model simulations.

In this study, we coupled the organic chemical modeling code PMOD, developed at LLNL, with a finite-element coupled fluid-flow and heat-transfer code developed at UC Berkeley to study and model how excess pore pressure is generated. The integrated code can be used to study how fluid pressures develop in areas such as the U.S. Gulf Coast, where excess pressure is commonly attributed to compaction disequilibrium, but where significant hydrocarbon resources have been discovered.

Progress

In FY 1992, we completed a finite-element program that couples thermal, hydrological, sedimentary, and organic geochemical processes in sedimentary basins. The program simultaneously calculates methane and CO₂ generation and their solubility in water, pore-pressure generation, and fluid transfer in an evolving basin. We tested the model using the Cascadia Basin off the Pacific Coast of Washington and Oregon, partly to investigate the resource potential of deep gas in this continental margin. The results of our study demonstrate that (1) methane and CO₂ show distinctly different timing in their formation, which leads to distinct spatial distributions; (2) sediment compaction is the dominant factor in the development of excess pore pressure, so methane and CO₂ production has little effect on pore pressures; and (3) an exceedingly low permeability seal is formed between the upper permeable turbidites and the lower impervious hemipelagites, beneath which high pore pressures can be maintained through geologic time. Our modeling was one dimensional; in FY 1993, we will extend it to two dimensions for broader applications.

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A significant improvement is the model's capability to handle the dynamic processes of hydrofracturing. Observations in sedimentary basins often show complex networks of veins, which preserve the evidence of repeated hydrofracturing, suggesting that fracture-dominated flow through rocks may be a crucial factor in the dispersion of pressurized fluids. We are perfecting the technique for modeling the processes of hydrofracturing when pore pressures exceed the local minimum principal stress. With this added capability to handle dynamic, transient processes, the program will be better equipped to study the aspect of hydrocarbon migration.

Cenozoic Volcanism and Crustal Evolution in Northern Mexico: Integrated Studies of Volcanic Rocks and Xenoliths

Principal Investigator: Ken Cameron (UC Santa Cruz)

LLNL Collaborator: Sidney Niemeyer

Student: David Kuentz (UC Santa Cruz)

Mid-Cenozoic volcanism in northern Mexico was the surface expression of a major pulse of crustal growth. Isotopic studies of lower and midcrustal mafic xenoliths and Cenozoic volcanic rocks establish that the crust beneath the region contains major (several kilometers thick), mafic layered intrusions where the differentiation of mid-Cenozoic magmas took place.

Abstract

Our objective is to construct and test an integrated model for the evolution of continental basaltic magmas, the formation of deep crust, and the genesis of voluminous Cenozoic rhyolites of northern Mexico. This model will be based on volcanic rocks that are typical of those erupted in the mid-Cenozoic in western North America, contemporaneous cumulates, wall rocks from various crustal levels, and compositions of uncontaminated primitive basaltic magmas determined from mantle xenolith studies.¹ The results have important implications regarding the amount of crustal growth that occurred in western North America during the Cenozoic.

Objectives

The late Cenozoic Camagaro basalt field, which lies in the Mexican state of Chihuahua about 500 km south-southeast of El Paso, Texas, contains at least 225 cinder cones and a few maar volcanoes. One of these cinder cones is the host for La Olivina xenolith locality.² We have searched about 10% of the veins in the basalt field and found significant numbers of xenoliths at about half of the sites. About half of these localities are dominated by extensively melted mafic to silicic xenoliths and are ignored here. The remaining localities fall into two main classes: (1) peridotite-dominated and (2) mafic-dominated.

The peridotite-dominated localities, including La Olivina, contain about 80% peridotite, 10% pyroxenite, and 10% granulites. The granulites are divided about equally among pelitic, mafic, and intermediate to silicic varieties. The mafic granulites contain plagioclase + orthopyroxene + clinopyroxene + spinel with minor amphibole in a few. In contrast, at the mafic-dominated localities, peridotite and paragneiss are rare or absent, and essentially all xenoliths are gabbroic in composition. Texturally and mineralogically, they range from anhydrous, two-pyroxene granulite, through hornblende granulite and pyroxene-bearing amphibolite assemblages, to amphibole-free rocks with igneous, orthocumulate textures. Xenoliths from mafic-dominated localities are interpreted to be from midcrustal levels, whereas those from peridotite-dominated localities are probably from the lower crust.

Rare-earth element and other trace-element data demonstrate that mafic rocks from both types of localities are cumulates, probably from magmas ranging from andesite to dacite or rhyolite in composition. The mafic granulites from La Olivina

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vary in $^{87}\text{Sr}/^{86}\text{Sr}$ from 0.7045 to 0.7057 and the fractional deviation from the isotopic composition of the chondritic Sm/Nd reservoir, ϵ_{Nd} , from 1.3 to -1 parts/ 10^4 . Five of the six analyzed xenoliths from mafic-dominated localities, including samples with the complete range in amphibole content, have less radiogenic strontium (0.7040 to 0.7043) than the mafic granulites from La Olivina.

The mafic xenoliths have much higher $^{87}\text{Sr}/^{86}\text{Sr}$ and lower ϵ_{Nd} than late Cenozoic basalts from the Camargo field (~ 0.7032 and ~ -4 , respectively). They are, however, similar in isotopic composition to middle Cenozoic andesite, dacite, and rhyolite lavas that crop out around the basalt field. These Tertiary volcanic rocks can be divided into two groups based on stratigraphy and trace-element compositions. Both have ϵ_{Nd} between about 2 and -1.5 , but the older (stratigraphically lower) group has lower initial $^{87}\text{Sr}/^{86}\text{Sr}$ (0.7040 to 0.7044) than the younger one (0.7045 to 0.7059). We interpret the xenoliths from mafic-dominated localities to be cumulates from magmas parental to the older volcanic group, whereas the mafic granulites from La Olivina are probably related to the younger group. The lower and middle crust beneath the region apparently contains major, mafic-layered intrusions where differentiation of middle Cenozoic magmas took place.

References

1. Nimz, G. J., K. L. Cameron, and S. Niemeyer (in press), "The La Olivina Pyroxenite Suite and the Isotopic Compositions of Mantle Basalts Parental to Mid-Cenozoic Arc Volcanism in Northern Mexico," *J. Geophys. Res.*
2. Cameron, K. L., J. V. Robinson, S. Niemeyer, G. J. Nimz, D. C. Kuentz, R. S. Harmon, S. R. Bohlen, and K. D. Collerson (in press), "Contrasting Styles of Pre-Cenozoic and Mid-Tertiary Crustal Evolution in Northern Mexico: Evidence from Deep Crustal Xenoliths from La Olivina," *J. Geophys. Res.*

Monazite Prograde Thermochronometry

Principal Investigators: T. Mark Harrison and Kevin D. McKeegan
(UC Los Angeles)

LLNL Collaborator: Frederick J. Ryerson

Students: William T. Akers and Marty Grove (UC Los Angeles)

The high retentivity of monazite for lead, its high uranium and thorium concentrations, and its emergence in staurolite zone metapelites suggest that it may be used as a prograde thermochronometer. However, the monazite-producing reactions in pelites are as yet incompletely understood. We have investigated the suggestion that rhabdophane, a light rare-earth element (LREE) $PO_4 \cdot H_2O$, may be an important reactant in monazite-producing reactions in pelitic compositions. Results of our combined hydrothermal and 0.1-MPa (1-bar) heating experiments preclude rhabdophane from being the immediate precursor to monazite in lower amphibolite facies metamorphic sequences and restrict rhabdophane occurrence to the uppermost portion of the crust. The low rhabdophane dehydration temperatures relative to the temperatures inferred for monazite formation in metapelites indicates that rhabdophane does not convert directly to monazite during pelite metamorphism. Rather, the monazite LREE component produced by rhabdophane breakdown must be incorporated in intermediate phases such as allanite and, perhaps more likely, LREE oxides prior to monazite formation.

Abstract

Our goal is to develop the monazite prograde thermochronometer. To accomplish this task, we require information from three distinct but related studies: (1) stability and reaction kinetics of LREE oxides and hydrous LREE phosphates in pelitic assemblages, (2) lead diffusion in monazite, and (3) development of U/Pb microanalysis of monazite. During FY 1992, we focused on the first of these studies.¹

Objectives

We performed a series of hydrothermal and 0.1-MPa (1-bar) heating experiments to establish the stability of rhabdophane and to determine whether rhabdophane is the immediate precursor to monazite in lower amphibolite facies metamorphic sequences. We analyzed run products using visible near-infrared spectroscopy (VNIRS) and x-ray diffraction (XRD). In all 22 hydrothermal runs in which rhabdophane was initially present, XRD analysis indicates that rhabdophane had completely dehydrated to monazite. At H_2O pressures of 50 to 200 MPa (500 to 2000 bar), therefore, rhabdophane is completely unstable relative to monazite at temperatures greater than 200°C.

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Dry, 0.1-MPa heating experiments indicate that La-rhabdophane persists (perhaps metastably) to temperatures approaching 500°C. XRD and VNIRS examination of La-rhabdophane heated isothermally in air at temperatures from 200 to 700°C indicates that structural water is largely retained up to 500°C for heating intervals of up to 24 hours. In the wavelengths between 900 and 2500 nm, untreated rhabdophane shows two sharp, well-defined absorbance features at 1450 and 1950 nm that represent molecular water situated within well-defined structural sites within the sample.² Structural modification involving H_2O appears to take place between 300 and 500°C; features of the two well-defined VNIRS bands remain sharp to 400°C but become progressively less pronounced and broader in

samples run at higher temperature. Partial decomposition of La-rhabdophane to La-monazite is observed at 600°C, and rapid and complete reaction to La-monazite occurs at 700°C.

Our results preclude rhabdophane from being the LREE precursor phase to monazite and thus suggest that another phase or phases may be the responsible agent. This conclusion is in accord with the findings of Kingsbury et al.,³ who found that the LREE in low-grade portions of the Bright Angel shale are contained in LREE oxide grains found mostly at the grain boundaries of major phases. Apatite may also be important. Monazite overgrowths on apatite have been found in higher-grade, monazite-bearing equivalents of Latham shale.³ These overgrowths suggest a possible monazite-forming reaction: apatite + LREE oxide = monazite + calcium-bearing phase.

Thus, we conclude that rhabdophane is unstable relative to monazite at temperatures less than at least 200°C for H₂O pressures of 50 to 200 MPa and oxygen fugacities imposed by the graphite-methane buffer. These findings make it unlikely that rhabdophane could be a reactant in monazite-producing reactions at the higher temperatures (~450 to 500°C) appropriate to the staurolite zone in pelitic sequences. We are investigating other phases to determine their possible roles as LREE or phosphorus-bearing precursors to monazite-forming reactions. LREE oxides and apatite show promise as the carrier phases for the monazite components in low-grade pelitic rocks.

References

1. Akers, W. T., M. Grove, T. M. Harrison, and F. J. Ryerson (in press), "The Instability of Rhabdophane and Its Unimportance in Monazite Paragenesis," *Chem. Geology*.
2. Hunt, G. R., J. W. Salisbury, and C. J. Lenhoff (1972), "Visible and Near-Infrared Spectra of Minerals and Rocks: V. Halides, Phosphates, Arsenates, Vanadates, and Borates," *Modern Geology* **3**, 121.
3. Kingsbury, J. A., C. D. Miller, J. L. Wooden, and T. M. Harrison (in press), "Monazite Paragenesis and U/Pb Systematics in Rocks of the Eastern Mojave Desert, California: Implications for Thermochronometry," *Chem. Geology*.

Section IV. IGPP-LLNL Workshops and Seminars

Center for High-Pressure Sciences

Seminars

October 17, 1991

“Structure-Property Relationships in Organic Aerogels”

Richard W. Pekala, Chemistry and Materials Science, LLNL

November 19, 1991

“Raman Studies on C₆₀ at High Pressures and Low Temperatures”

Sarah Tolbert, UC Berkeley

November 21, 1991

“Quantum Monte Carlo Studies of Hydrogen and Helium”

Karl Runge, CP Division, LLNL

November 22, 1991

“Synthesis and Processing of Ceramic Materials”

Joanna McKittrick, UC San Diego

December 9, 1991

“Hydrothermal Studies in the Diamond Anvil Cell: The Equation of State of Water”

William B. Bassett, Cornell University, Ithaca, NY

December 12, 1991

“Fractured Statistics: Theory vs Experiment”

Robert Laughlin, H Division, LLNL

December 13, 1991

“Experimental Constraints on the Metallization of Hydrogen”

Russ Hemley, Carnegie Institute of Washington, Geophysical Library

December 17, 1991

“Optical Measurements of Simple Systems at High Pressures: Hydrogen and Argon”

Hector Lorenzana, UC Berkeley

January 16, 1992

“Three-Dimensional Analog of Anyons and Superconductivity”

Stephen B. Libby, A Division, LLNL

January 31, 1992

“Formation of Tektites by Multiple Impacts”

John Wasson, UC Los Angeles

February 7, 1992

"Pressure-Induced Amorphization"

Ray Jeanloz, UC Berkeley

February 13, 1992

"Phase Relations in the Diamond Anvil Cell"

Malcolm Nicol, UC Los Angeles

February 20, 1992

"Surface Structure Determination Using Photoelectron Holography"

Lou J. Terminello, Chemistry and Materials Science, LLNL

February 27, 1992

"Phase Transformations in Perovskite Viewed in the TEM plus Anisotropic
Convection in the Upper Mantle"

Hans-Rudolf Wenk, UC Berkeley

March 3, 1992

"Shock Deformation and Transformation of Sapphire"

David Howitt, UC Davis

March 6, 1992

"In Situ Observations of Microstructures during Shock Loading"

Alan Frank, B Division, LLNL

March 12, 1992

"Nonclassical Nucleation in Fluid to Solid Phase Transitions"

William Klein, Boston University, MA

March 13, 1992

"In Situ Observations of Microstructures during Shock Loading"

Alan Frank, B Division, LLNL

March 27, 1992

"Theory of STM from Clean and Adsorbate-Covered Metal Surfaces"

Dejana Drakova, University of Sofia, Bulgaria

April 1, 1992

"Impact Delivery of Organics to the Early Earth"

Leigh Brookshaw, IGPP-LLNL

April 2, 1992

"The Glass Transition in Polymeric Systems"

Dieter Heerman, Institut für Theoretische

April 3, 1992

"Materials Studies Utilizing the Shock Compression Technique in the Japanese
Inter-University Program"

Akira Sawaoka, Tokyo Institute of Technology, Japan

April 9, 1992

"Angle-Resolved Photoemission from the Normal and Superconducting States of
the Cuprate Superconductors"

Daniel Dessau, Stanford University, Palo Alto, CA

April 10, 1992

“Pressure-Induced Collapse of the Tetragonal Framework in Silicates and Germanates”

George Wolf, Arizona State University, Tempe

April 17, 1992

“High-Pressure Sintering and Deformation of Silica Aggregates”

Mark Beeman, Earth Sciences, LLNL

April 17, 1992

“Friction Force Microscopy on Langmuir–Blodgett Film”

Ernst Meyer, University of Basil, Switzerland

April 17, 1992

“Giant Magnetoresistance and Antiferromagnetic Interlayer Coupling in Ferromagnet/Paramagnet Multilayers”

Ernst Meyer and Rene Orderny, University of Basil, Switzerland

April 22, 1992

“Computer Simulations of Fragmentation”

H. J. Melosh, Arizona State University, Tempe

April 23, 1992

“Giant Magnetoresistance and Antiferromagnetic Interlayer Coupling in Ferromagnet/Paramagnet Multilayers”

Allison Chaiken, Chemistry and Materials Science, LLNL

April 29, 1992

“High-Pressure Sintering and Deformation of Silica Aggregates”

Mark Beeman, Earth Sciences, LLNL

April 30, 1992

“Mechanical Instability in Some Supercooled Liquids”

Pablo DeBenedetti, UC Berkeley

May 12, 1992

“Molecular Computers”

Tom Rust, Lazerus Computing

May 15, 1992

“Application of Kohn–Sham Formalism to Quantum Dots with Realistic Dimension”

Ching Y. Fong, UC Davis

June 11, 1992

“Solid Hydrogen at High Pressure: Modeling of Dielectric Properties”

Alberto Garcia, UC Berkeley

June 25, 1992

“A Molecular Dynamics Simulation of Wearless Friction between Ordered Films of Short Organic Chains”

James Glosli, IBM Almaden Research, San Jose, CA

June 29, 1992

“Ab Initio Studies on High-Pressure Phase of Ice”

Changyol Lee, Harvard University, Cambridge, MA

July 23, 1992

“Interatomic Potentials from Sub-Doppler Lineshapes”

Kurt Gobble, Stanford University, Palo Alto, CA

August 3, 1992

“Partially Ionized Dense Plasmas: Theory of Equilibrium and Nonequilibrium Properties”

Wolf Kraeft, University of Greifswald, Germany

August 13, 1992

“Materials by Computer Design”

Christian Mailhot, H Division, LLNL

August 21, 1992

“The Paired-Electron Crystal”

Neil Ashcroft, Cornell University, Ithaca, NY

August 27, 1992

“Theoretical Studies of Fluorine and Hydrogen Interactions with Silicon (100) Surfaces”

Christine Jiang Wu, UC Los Angeles

September 10, 1992

“Catastrophe Disruption: From Laboratory Experiments to Asteroid Impacts”

Eileen Ryan, University of Arizona, Tucson

Astrophysics Research Center

Workshop

March 24, 1992

Geodesy Workshop at IGPP-LLNL

Hosted by John Rundle

Seminars

October 4, 1991

“Optical Signatures of Cooling Flows in Elliptical Galaxies”

Susana Deustua, IGPP-LLNL

October 11, 1991

“Cosmological Implications of Whole-Sky Redshift Surveys”

Marc Davis, UC Berkeley

October 18, 1991

“A Compton Reflection Model for the Cosmic X-Ray and Gamma-Ray Background”

Robert Rogers, IGPP-LLNL

October 25, 1991

“Shock Precursors and the Onset of Cooling behind Fast Shocks in the Cygnus Loop”

Jeff Hester, Arizona State University, Tempe

October 28, 1991

“On Protons and Dileptons as Signals of the Quark–Gluon Plasma”

Dinesh Srivastava, Variable Energy Cyclotron Center, Calcutta, India

November 1, 1991

“Astrophysical Hot Hydrogen Burning Reaction Rates”

Pierre Auger, Laboratoire des Spectrometrie, Orsay, France

November 5, 1991

“High-Pressure and Magnetic Relaxation Measurements on

$Y_{1-x}Pr_xBa_2Cu_3O_7$ ”

Lisa Paulius, UC San Diego

November 7, 1991

“Early Stages of Terrestrial Planet Formation”

Glenn Stewart, University of Colorado, Boulder

November 8, 1991

“First Results from the Compton Gamma-Ray Observatory”

Neil Gehrels, NASA, Goddard Space Flight Center, Greenbelt, MD

November 15, 1991

“An Obstacle to Building a Time Machine”

Alan Guth, Massachusetts Institute of Technology, Cambridge

November 22, 1991

“Barium Stars and Related Binaries”

Peter Eggleton, Institute of Astronomy, Cambridge, England

November 26, 1991

“A Self-Consistent Theory of Collisionless Relaxation: How to Find Globally Stable Final States”

Heinz Wiechen, Ruhr Universitat, Doctum, Germany

December 3, 1991

“Recent ROSAT Observations of X-Ray Sources”

Tomaso Belloni, Max Planck Institute, Garching, Germany

December 6, 1991

“‘Hidden’ Millisecond Pulsars: A New Class of Gamma-Ray Sources”

Marco Tavani, IGPP-LLNL

December 13, 1991

“Magnetic Fields in Star-Forming Regions”

Ellen Zweibel, University of Colorado, Boulder

December 20, 1991

“New Results from GRO”

Edison Liang, Rice University, Houston, TX

January 10, 1992

“Shells, Supershells, Worms, and Chimneys in the Interstellar Medium”

Carl Heiles, UC Berkeley

January 17, 1992

“Planet Formation”

Jack Lissauer, State University of New York, Stony Brook

January 24, 1992

“Low-Surface Brightness Galaxies”

Greg Bothun, University of Oregon, Eugene

January 31, 1992

“A Magnetically Heated Galactic Halo”

John Raymond, Center for Particle Astrophysics

February 7, 1992

“ROSAT Observations of Supernova Remnants and the Interstellar Medium”

Bernard Aschenbach, Max-Planck-Institut für Extraterrestrische Physik

February 14, 1992

“UV Pulsations from Massive X-Ray Binaries”

Tim Kallman, NASA, Goddard Space Flight Center, Greenbelt, MD

February 18, 1992

“Type I Supernovae and the Duration of the Formation of the Galactic Stellar Halo”

Tammy A. Smecker, Johns Hopkins University, Baltimore, MD

February 19, 1992

“New Approach to Determining the Gruneisen Parameter”

Orson Anderson, UC Los Angeles

February 21, 1992

“Lyman- α Clouds as a Probe of the Intergalactic Medium”

Jane C. Charlton, University of Arizona, Tucson

February 21, 1992

“Observations and Theory of Stellar Flares”

Suzanne Hawley, IGPP–LLNL

February 28, 1992

“Direct Measurements of Stellar Magnetic Fields”

Gibor Basri, UC Berkeley

March 6, 1992

“Very Long Baseline Infrared Interferometry”

Bill Danchi, Space Sciences Laboratory, UC Berkeley

March 12, 1992

“Is Inflation Fine-Tuned?”

Bharat Ratra, California Institute of Technology, Pasadena

March 13, 1992

“Pre–White Dwarf Evolution”

Volker Weidemann, Institut für Theoretische Physik and Sternwarte der Universität
Kiel, Germany

March 20, 1992

“Large-Scale Structure in the Northern Sky”

Stephane Courteau, Cornell University, Ithaca, NY

March 27, 1992

“ROSAT X-Ray Observations and the Stellar Coronal Dividing Line”

Bernard Haisch, Lockheed, Palo Alto Research Laboratory, CA

April 3, 1992

“What Regulates Star Formation in Galaxies?”

Robert Kennicutt, Steward Observatory, University of Arizona, Tucson

April 10, 1992

“Starburst-Driven Galactic Superwinds”

Timothy Heckman, Space Telescope Science Institute and Johns Hopkins
University, Baltimore, MD

April 17, 1992

“The Tully–Fisher Relation Using CO Emission Lines”

John Dickey, University of Minnesota

April 24, 1992

“A Comparison of the Atmosphere–Surface Relationships between Mercury
and the Moon”

Ann Sprague, Lunar and Planetary Laboratory, University of Arizona, Tucson

April 29, 1992

“High-Pressure Sintering and Deformation of Silica Aggregates”

Mark Beeman, Earth Sciences, LLNL

May 1, 1992

“Measuring the Universe with Supernovae”

Robert Kirshner, Harvard University, Cambridge, MA

May 8, 1992

“Cosmological Evolution of Accretion Disks and Quasars”

Vahe Petrosian, Stanford University, Palo Alto, CA

May 15, 1992

“The Galaxy at Faint Magnitudes: Constraints on the Evolution of the Milky Way”

Steven Majewski, Observatories of the Carnegie Institute of Washington

May 22, 1992

“The Las Campanas Fiber-Optic Redshift Survey: The End of Large-Scale Structure”

Stephen Sheckman, Observatories of the Carnegie Institute of Washington

May 29, 1992

“Rocket-Borne Observations of [CII] 158- μ m Emission from the Diffuse Interstellar Medium”

Jamie Bock, UC Berkeley

June 5, 1992

“COBE Observations of the Anisotropy of the Cosmic Microwave Background”

Charles Lineweaver, Lawrence Berkeley Laboratory, CA

June 12, 1992

“Signal Detection and Supercomputing in the Search for Extraterrestrial Intelligence”

Kent Cullers, NASA-Ames Research Center, Moffett Field, CA

June 18, 1992

“BATSE Observations of Gamma-Ray Bursts”

David Band, Center for Astrophysics and Space Science, UC San Diego

June 19, 1992

“Comets, Craters, and Catastrophes”

Eugene Shoemaker, U.S. Geological Survey, Menlo Park, CA

June 26, 1992

“A Large Arc near the Double Quasar 0957+561: Gravitational Lensing, Dark Matter, and the Hubble Constant”

Gary Bernstein, University of Arizona, Tucson

July 10, 1992

“Nuclear Interaction Rates for Dark Matter Detectors”

Ted Russell, IGPP-LLNL

July 17, 1992

“Initial Observations of the Solar Corona from Yohkon”

Keith Strong, Lockheed, Palo Alto Research Laboratory, CA

July 22, 1992

“Type II Supernovae and the Equation of State of Dense Matter”

F. D. Swesty, State University of New York, Stony Brook

July 24, 1992

“Magnetic Fields in Clusters of Galaxies”

Yoel Rephaeli, UC San Diego

July 31, 1992

“Mass Loss from Cool Evolved Stars”

Chris Skinner, UC Berkeley-IGPP Laboratory for Experimental Astrophysics

August 7, 1992

“IRAS Images and the History of Variable Mass Loss from Red Giant Stars”

George Hawkins, IGPP–LLNL

August 14, 1992

“Topics in Gamma-Ray Astrophysics”

Edison P. Liang, Rice University, Houston, TX, and LLNL

August 21, 1992

“High Spectral Resolution Gamma-Ray Observations on the Galactic Center Region”

Bob Lin, UC Berkeley

August 27, 1992

“Starburst-Driven Superwinds”

Matthew D. Lehnert, Johns Hopkins University, Baltimore, MD

August 28, 1992

“New News about Nu’s”

Sidney Bludman, University of Pennsylvania, Philadelphia, and Center for Particle Astrophysics

September 4, 1992

“The Puzzle of Giant Ionized Gas Filaments in Irregular Galaxies”

Diedre Hunter, Lowell Observatory

September 11, 1992

“Neutrino Oscillations, Closure Mass Neutrinos, and Supernovae”

George Fuller, UC San Diego

September 18, 1992

“Millimeter-Wave Measurements of the Sunyaev–Zel’dovich Effect: A New Tool for Observational Cosmology”

Marc Fischer, UC Berkeley

September 25, 1992

“A Random Walk through the Solar Corona”

Tim Bastian, NRAO/VLA

Center for Geosciences

Seminars

October 7, 1991

“Phenomenological Approach to Unsaturated Flow of Non-Newtonian Solutions in Soils and Porous Media”

John Philip, CSIRO Centre for Environmental Mechanics, Australia

October 14, 1991

“Applications of Shallow Seismic Reflection to Environmental and Engineering Problems”

Donald Steeples, Kansas Geological Survey, Lawrence

November 8, 1991

“Permeability of Sandstones from Image Processing”

Stephen Blair, Earth Sciences, LLNL

November 21, 1991

“An Inversion of Seismic Refraction-Line First Arrival Times”

Chuck Ammon, UC Santa Cruz

November 21, 1991

“Inversion Strategies at a Geologically Complex Plate Boundary: Characterizing Fault Slip in Southern California from Geodetic Data”

Hadley Johnson, Scripps Institute of Oceanography, UC San Diego

December 6, 1991

“A Geochemical Transport Model for Redox-Controlled Movement of Mineral Fronts in Groundwater Flow Systems: Denitrification by Oxidation of Pyrite”

Ken Kipp, U.S. Geological Survey, Denver, CO

December 16, 1991

“NMR Investigations of the Interaction of Water with Minerals and Glasses”

R. James Kirkpatrick, University of Illinois, Urbana-Champaign

December 16, 1991

“Neutral Buoyancy Magma Transport in Volcanic Rift Zones”

Mike Ryan, U.S. Geological Survey, Reston, VA

December 16, 1991

“The Path of the Pole during Geomagnetic Reversals”

Stanley Runcorn, University of Alaska

December 17, 1991

“Seismic Velocities in Compacting Sediments”

Jack Dvorkin, Stanford University, Palo Alto, CA

February 14, 1992

“Liquid Fuels in the 21st Century: A Nuclear Option”

Donald Towse, Earth Sciences, LLNL

February 25, 1992

“Two Topics in Fault Dynamics: Experimental Observations of Interface Separation Waves during Stick Slip and a Cellular Automation Model of Earthquakes”

Stephen R. Brown, Sandia National Laboratories, Albuquerque, NM

March 11, 1992

“Petrologic Applications of Single and Double Medium Diffusion Modeling”

Herb Wang, University of Wisconsin, Madison

March 23, 1992

“Katmai Scientific Drilling Project: Results and Outlook”

John Eichelberger, University of Alaska

April 8, 1992

“Effects of Defects on Electrical Properties of Olivine”

Barbara J. Wanamaker, University of Minnesota

April 28, 1992

“A Fractal Analysis of Sea-Level Changes—Implications for Global Change”

Albert T. Hsui, University of Illinois, Urbana

May 1, 1992

“North Sea Clastic Diagenesis and Formation Water Constraints”

Per Aagaard, University of Oslo, Norway

July 8, 1992

“Experimental Deformation of a Quartz Mylonite: The Influence of Chemical Environment, or Wet about the Ears with Quartz Deformation”

James N. Boland, Division of Geomechanics, CSIRO, Australia

August 10, 1992

“Radionuclides Migration at MAYAK in Russia”

Igor Khodakovsky, Russian Academy of Sciences, Moscow

August 12, 1992

“Modeling Compaction and Dilation of Porous Rocks”

Miles Rubin, Technion—Israel Institute of Technology

September 24, 1992

“Deformation during a Solid-State Phase Transformation and the Influence of an Externally Applied Axial Stress—Geophysical and Technological Implications”

Alex McLaren, Australian National University, Canberra

Section V. Bibliography

1992

Anderson, O. L., D. Isaak, and H. Oda (1992), "High-Temperature Elastic Constant Data on Minerals Relevant to Geophysics," *Rev. Geophys.* **30**, 57.

Arons, J. (1992), "Magnetospheres of Rotation-Powered Pulsars," in *Magnetospheric Structure and Emission Mechanisms of Radio Pulsars, Proc. IAU Colloq. No. 128*, T. H. Hankins, J. M. Rankin, and J. Gil, Eds. (Pedagogical University Press, Zielona Gora), p. 56.

Arons, J. (1992), "Photon Bubbles: Overstability in a Magnetized Atmosphere," *Astrophys. J.* **388**, 561.

Arons, J. (in press), "Relativistic Shock Waves and the Excitation of Plerions," in *Collective Acceleration Processes in Collisionless Plasmas*, D. Le Queau, Ed. (Les Editions de Physique, Paris).

Arons, J. (1992), "Relativistic Shock Waves and the Excitation of Plerions," in *X-Ray Binaries and the Formation of Binary and Millisecond Radio Pulsars*, E. P. J. van den Heuvel and S. A. Rappaport, Eds. (Kluwer, Boston), p. 361.

Arons, J., Y. Gallant, M. Hoshino, A. B. Langdon, and C. E. Max (1992), "Relativistic Shocks and the Excitation of Plerions," in *Magnetospheric Structure and Emission Mechanisms of Radio Pulsars, Proc. IAU Colloq. No. 128*, T. H. Hankins, J. M. Rankin, and J. Gil, Eds. (Pedagogical University Press, Zielona Gora), p. 78.

Ball, R. (1992), "A Dynamical Analysis of the Barred Spiral Galaxy NGC 3359," *Astrophys. J.* **395**, 418.

Ball, R., J. Arens, G. Jernigan, E. Keto, and M. Meixner (1992), "Thermal Dust Imaging: The Onset of Asymmetry in the Ultracompact HII Region," *Astrophys. J.* **389**, 616.

Baum, S. A., T. M. Heckman, and W. van Breugel (1992), "Spectroscopy of Emission-Line Nebulae in Powerful Radio Galaxies: Interpretation," *Astrophys. J.* **389**, 208.

Becker, R. H., D. J. Helfand, and R. L. White (1992), "The Discovery of an X-Ray Selected, Radio-Loud Quasar at $z = 3.9$," *Astron. J.* **104**, 531.

Becker, R. H., R. L. White, and D. D. Proctor (1992), "A Serendipitous Survey of the Galactic Plane for Type II OH Masers," *Astron. J.* **103**, 544.

Bennet, D., A. Stebbins, and F. Bouchet (1992), "The Implications of the COBE Diffuse Microwave Radiation Result for Cosmic Strings," *Astrophys. J. Lett.* **399**, L5.

- Benz, H. M., G. Zandt, and D. H. Oppenheimer (1992), "Lithospheric Structure of Northern California from Teleseismic Images of the Upper Mantle," *J. Geophys. Res.* **97**, 4791.
- Cameron, K. L., J. V. Robinson, S. Niemeyer, G. J. Nimz, D. C. Kuentz, R. S. Harmon, S. R. Bohlen, and K. D. Collerson (1992), "Contracting Styles of Pre-Cenozoic and Mid-Tertiary Crustal Evolution in Northern Mexico: Evidence from Deep Crustal Xenoliths from La Olivina," *J. Geophys. Res.* **97**, 17353.
- Carrigan, C. R., G. Schubert, and J. C. Eichelberger (1992), "Thermal and Dynamical Regimes of Single and Two-Phase Magmatic Flow in Dikes," *J. Geophys. Res.* **97**, 17377.
- Constable, S., T. J. Shankland, and A. Duba (1992), "The Electrical Conductivity of an Isotropic Olivine Mantle," *J. Geophys. Res.* **97**, 3397.
- Cynn, H., S. K. Sharma, T. F. Cooney, and M. Nicol (1992), "High-Temperature Raman Investigation of Order-Disorder Behavior in MgAl_2O_4 Spinel," *Phys. Rev. B* **45**, 500.
- Duba, A. G. (1992), "Geophysics: Earth's Core Not so Hot," *Nature* **359**, 197.
- Duba, A. G., and S. Constable (1992), "Comparison of Electrical Conductivity of Single Crystal Olivine, Dunite, and Lherzolite," (submitted).
- Duong, H., M. Beeman, and J. Wolfenstine (1992), "Creep of KCl-KBr Solid Solution Alloys," *J. Mater. Sci. Lett.* **11**, 238.
- Durham, W. B., S. H. Kirby, and L. A. Stern (in press), "Rheologies of Ice I: The Effect of Particulate Impurities and Initial Grain Size," *J. Geophys. Res.*
- Filippenko, A. V., M. W. Richmond, D. Branch, C. M. Gaskell, W. Herbst, C. H. Ford, R. R. Treffers, T. Matheson, L. C. Ho, A. Dey, W. L. W. Sargent, T. A. Small, and W. J. M. van Breugel (1992), "The Subluminous, Spectroscopically Peculiar Type Ia Supernova 1991bg in the Elliptical Galaxy NGC 4374," *Astron. J.* **104**, 1543.
- Freeman, W. L., B. F. Madore, S. L. Hawley, I. K. Horowitz, J. Mould, M. Navarrete, and S. Sallmen (1992), "New Cepheid Distances to Nearby Galaxies Based on BVRI CCD Photometry. III. NGC 300," *Astrophys. J.* **396**, 80.
- Fuller, G., R. Mayle, B. Meyer, and J. Wilson (1992), "Can a Closure Mass Neutrino Help Solve the Supernova Shock Reheating Problem?" *Astrophys. J.* **389**, 517.
- Gallant, Y., M. Hoshino, A. B. Langdon, J. Arons, and C. E. Max (1992), "Relativistic, Perpendicular Shocks in Electron-Positron Plasmas," *Astrophys. J.* **391**, 73.
- Goldstein, P., W. Walter, and G. Zandt (1992), "Upper-Mantle Structure beneath Central Eurasia Using a Source Array of Nuclear Explosions and Waveforms at Regional Distances," *J. Geophys. Res.* **97**, 14097.

- Goodman, C. D., M. B. Aufderheide, S. D. Bloom, and D. A. Resler (1992), "Comments on 'Is the Weak Axial-Vector Current Renormalized in Nuclei?' " *Phys. Rev. Lett.* **69**, 2445.
- Harrison, M., C. Wenji, P. H. Leloup, F. J. Ryerson, and P. Tapponnier (1992), "An Early Miocene Transition in Deformation Regime within the Red River Fault Zone, Yunnan, and Its Significance for Indo-Asian Tectonics," *J. Geophys. Res.* **97**, 7159.
- Hawley, S. L., and G. H. Fisher (1992), "X-Ray-Heated Models of Stellar Flare Atmospheres: Theory and Comparison with Observations," *Astrophys. J. Suppl.* **81**, 885.
- Helfand, D. L., S. Zoonematkermani, R. H. Becker, and R. L. White (1992), "Compact Radio Sources near the Galactic Plane," *Astrophys. J. Suppl.* **80**, 211.
- Hoshino, M., J. Arons, Y. Gallant, and A. B. Langdon (1992), "Relativistic Magnetosonic Shock Waves in Synchrotron Sources: Shock Structure and Non-Thermal Acceleration of Positrons," *Astrophys. J.* **390**, 454.
- Kawano, L. H., G. M. Fuller, R. A. Malaney, and M. J. Savage (1992), "Limits on Magnetic Moments of Heavy Neutrinos from Nucleosynthesis," *Phys. Lett. B* **275**, 487.
- Keto, E., R. Ball, J. Arens, G. Jernigan, and M. Meixner (1992), "Mid-Infrared Imaging of Markarian 231 and Arp 220," *Astrophys. J. Lett.* **387**, L17.
- Keto, E., R. Ball, J. Arens, G. Jernigan, and M. Meixner (1992), "Subarcsecond Mid-Infrared Imaging of the Nuclei of the Infrared Bright Galaxies NGC 1614 and NGC 7469," *Astrophys. J.* **389**, 223.
- Keto, E., D. Proctor, R. Ball, J. Arens, and G. Jernigan (1992), "The Environments of Young Stars: Mid-Infrared and Molecular Line Imaging," *Astrophys. J. Lett.* **401**, L113.
- Kirby, S. K., W. B. Durham, and L. A. Stern (1992), "The Ice I $\rightarrow$ II Transition: Mechanics and Kinetics under Hydrostatic and Nonhydrostatic Conditions," in *Physics and Chemistry of Ice*, N. Maeno and T. Hondoh, Eds. (Sapporo, Japan), p. 456.
- Li, X., L. C. Ming, M. H. Manghnani, Y. Wang, and R. Jeanloz (1992), "Pressure Dependence of the Electrical Conductivity of $\text{Mg}_9\text{Fe}_{0.1}\text{SiO}_3$ Perovskite," *J. Geophys. Res.* (submitted).
- Liedahl, D. A., S. M. Kahn, A. L. Osterheld, and W. H. Goldstein (1992), "X-Ray Emission-Line Spectra of Photoionized Plasmas: Density Sensitivity of the Fe L-Shell Series," *Astrophys. J.* **391**, 306.
- Lindley, G., and R. Archuleta (1992), "Earthquake Source Parameters and the Frequency Dependence of Attenuation at Coalinga, Mammoth Lakes, and the Santa Cruz Mountains, California," *J. Geophys. Res.* **97**, 14137.

- Mathews, G. J., G. Bazan, and J. J. Cowan (1992), "Evolution of Heavy-Element Abundances as a Constraint on Sites for Neutron-Capture Nucleosynthesis," *Astrophys. J.* **391**, 719.
- McKittrick, J., B. Tunaboylu, J. D. Katz, and W. Nellis (1992), " $\text{Al}_2\text{O}_3\text{-ZrO}_2$ Ceramics with Submicron Microstructures Obtained through Microwave Sintering, Plasma Sintering, and Shock Compaction," *Mater. Res. Soc.* **274**, 149.
- Meyer, B. S., G. J. Mathews, W. M. Howard, S. E. Woosley, and R. D. Hoffman (1992), "r-Process Nucleosynthesis in the High-Entropy Supernova Bubble," *Astrophys. J.* **399**, 656.
- Miley, G. K., K. C. Chambers, W. J. M. van Breugel, and F. Macchetto (1992), "Hubble Space Telescope Imaging of Distant Galaxies: 4C 41.17 at $z = 3.8$," *Astrophys. J. Lett.* **401**, L69.
- Moran, E. C., J. P. Halpern, G. D. Bothun, and R. H. Becker (1992), "Was 49: Mirror for a Hidden Seyfert 1 Nucleus?" *Astron. J.* **104**, 990.
- Nellis, W. J., A. C. Mitchell, P. C. McCandless, D. Erskine, and S. T. Weir (1992), "Electronic Energy Gap of Molecular Hydrogen from Electrical Conductivity Measurements at High Shock Pressures," *Phys. Rev. Lett.* **68**, 2937.
- O'Dea, C. P., S. A. Baum, C. Stanghellini, A. Dey, W. van Breugel, S. Duestua, and E. P. Smith (1992), "Radio and Optical Observations of 0218+357: The Smallest Einstein Ring?" *Astron. J.* **104**, 1320.
- Pettersson, B. R., S. L. Hawley, and G. H. Fisher (1992), "Starspots: The Zebra Effect," *Solar Phys.* **142**, 197.
- Skinner, C. J., A. G. G. M. Tielens, M. J. Barlow, and K. Justtanont (1992), "Methanol Ice in the Protostar GL 2136," *Astrophys. J. Lett.* **399**, L79.
- Tavani, M. (1992), "Pulsar-Irradiated Stars in Dense Globular Cluster," *Astron. Astrophys.* **261**, 472.
- Tavani, M., and L. Brookshaw (1992), "Planetary Systems around Millisecond Pulsars," *Nature* **356**, 320.
- Tolbert, S. H., A. P. Alivisatos, H. E. Lorenzana, M. B. Kruger, and R. Jeanloz (1992), "Raman Studies on C_{60} at High Pressures and Low Temperatures," *Chem. Phys. Lett.* **188**, 163.
- van Breugel, W. J. M., and A. Dey (1992), "Induced Star Formation in a Radio Lobe of 3C 285," *Astrophys. Lett.* (submitted).
- van Breugel, W. J. M., C. Fanti, R. Fanti, C. Stanghellini, R. T. Schilizzi, and R. E. Spencer (1992), "Compact Steep-Spectrum 3 CR Sources: VLA Observations at 1.5, 15, and 22.5 GHz," *Astron. Astrophys.* **256**, 56.
- Vidale, J., and H. M. Benz (1992), "Upper-Mantle Seismic Discontinuities and the Thermal Structure of Subduction Zones," *Nature* **356**, 678.

White, R., and R. Becker (1992), "A New Catalog of 30,239 1.4-GHz Sources," *Astrophys. J.* **388**, 220.

White, R., and R. Becker (1992), "Compact Radio Sources near the Galactic Plane," *Astrophys. J.* **388**, 221.

Woosley, S. E., and R. D. Hoffman (1992), "The α -Process and the γ -Process," *Astrophys. J.* **395**, 202.

1991

Bennett, D. P., and F. R. Bouchet (1991), "Constraints on the Gravity-Wave Background Generated by Cosmic Strings," *Phys. Rev. D* **43**, 2733.

Steck, L. (1991), *Array Analysis of 3-Component Teleseismic P and P-Coda Waves for Crustal Structure at Long Valley Caldera, California*, Ph.D. thesis, University of California at Santa Barbara.

Wenk, H.-R. (1991), "Standard Project for Pole Figure Determination by Neutron Diffraction," *J. Appl. Cryst.* **24**, 920.

1990

Drake, T. G. (1990), "Structural Features in Granular Flows," *J. Geophys. Res.* **95**, 8681.

Nelson, G. D., and J. E. Vidale (1990), "Earthquake Locations by 3-D Finite-Difference Travel Times," *Bull. Seis. Soc. Am.* **80**, 395.

Section VI. Fiscal Year 1993 IGPP-LLNL University Collaborative Research Program

Project No.	Principal investigator	University affiliation	LLNL collaborator	Project title
AP-93-05	Hyron Spinrad	UC Berkeley, Astronomy Dept.	Wil van Breugel	Optical Properties of Nearby Radio Galaxies
AP-93-07	James Graham	UC Berkeley, Space Sciences Laboratory	Christopher Skinner	An Observational Study of Evolved Stars and Planetary Nebulae
AP-93-08	Oswald Siegmund	UC Berkeley, Space Sciences Laboratory	Christopher Mauche	EUV Observations of Cataclysmic Variables with EUVE and ALEXIS
AP-93-11	Stanford Woosley	UC Santa Cruz, Lick Observatory	Grant Mathews	The r-Process in Supernovae and Accretion-Induced Collapse
AP-93-12	Jonathan Arons	UC Berkeley, Theoretical Astrophysics Center	Bruce Langdon	The Excitation of the Crab Nebula
AP-93-13	Gibor Basri	UC Berkeley, Astronomy Dept.	Suzanne Hawley	Hamilton Echelle Spectroscopy of Solar Flares
AP-93-16	Christopher Stubbs	UC Santa Barbara, Physics Dept.	Charles Alcock	Design Study for a Survey for Earth-Crossing Asteroids
AP-93-17	Philip Lubin	UC Santa Barbara, Physics Dept.	David Bennett	Cosmic Microwave Background Constraints on the Global Monopole and Texture Models of Cosmic Structure Formation
AP-93-19	Stanley Flatte	UC Santa Cruz, Institute of Tectonics	Claire Max	Atmospheric Characterization for Adaptive Optics
AP-93-22	George Fuller	UC San Diego, Physics Dept.	Grant Mathews	The Relationship between Supernova Dynamics and Nucleosynthesis and Closure Mass Neutrinos
GC-93-24	Mark Harrison	UC Los Angeles, Earth and Space Sciences Dept. and IGPP	Rick Ryerson	Monazite as a Thermochronometer for Prograde Metamorphism
GC-93-26	Steven Constable	UC San Diego, Scripps Institute of Oceanography	Al Duba	The Electrical Properties of a Mantle Rock

Fiscal Year 1993 IGPP-LLNL University Collaborative Research Program

Project No.	Principal investigator	University affiliation	LLNL collaborator	Project title
GC-93-29	Devendra Lal	UC San Diego, Scripps Institute of Oceanography	Marc Caffee	A Critical Test of the Applicability of $^{10}\text{Be}/^9\text{Be}$ Ratios in Authigenic Minerals for Determining Soil Formation Rates
GC-93-31	James R. Boles	UC Santa Barbara, Geological Sciences Dept.	Carol Bruton	Effect of Petroleum on Sandstone Reservoirs, San Joaquin Basin, California
GC-93-33	Quentin Williams	UC Santa Cruz, Institute of Tectonics	Rick Ryerson	Element Partitioning at High Pressures between Model Peridotites and Carbonate-Bearing Melts: Constraints on Deep-Earth Metasomatic Processes
GC-93-34	William Dietrich	UC Berkeley, Geology and Geophysics Dept.	Bryant Hudson	Cosmogenic Isotopes Applied to the Development of Longitudinal Profiles in Bedrock
GC-93-36	Aristides Yayanos	UC San Diego, Scripps Institute of Oceanography	William Bourcier	Microbial Mediation of Glass Alteration: Rates and Mechanisms
GP-93-39	Craig Nicholson	UC Santa Barbara, Institute for Crustal Studies	Jay Zucca	Subsurface Imaging of Velocity Structure within the Salton Sea Geothermal Area Using High-Resolution Tomography
GP-93-40	David Jackson	UC Los Angeles, Earth and Space Sciences Dept.	John Rundle	Models for Long-Term Earthquake Correlations
GP-93-41	Louise Kellogg	UC Davis, Geology Dept.	John Rundle	Global Positioning System Measurement of the White Wolf Fault, Greater Los Angeles Region
GP-93-42	Susan Schwartz	UC Santa Cruz, Institute of Tectonics	George Zandt	Determination of Three-Dimensional Velocity Variations in the Crust and Upper Mantle beneath Costa Rica
GP-93-43	Charles Ammon	UC Santa Cruz, Institute of Tectonics	Howard Patton	The Lithospheric Structure beneath the Western United States from the Inversion of Surface-Wave Phase-Velocity Measurements

Fiscal Year 1993 IGPP-LLNL University Collaborative Research Program

Project No.	Principal investigator	University affiliation	LLNL collaborator	Project title
GP-93-44	J.-B. Minster	UC San Diego, Scripps Institute of Oceanography	Howard Patton	Determination of Detailed Crust and Upper-Mantle Structure beneath a Three-Component, Broadband Small-Aperture Array
GP-93-45	Jiajun Zhang	UC Santa Cruz, Institute of Tectonics	William Walter	Shear-Wave Velocity Structure beneath Central California from Surface-Wave Dispersion
GP-93-46	Barbara Romanowicz	UC Berkeley, Seismographic Station	Kevin Mayeda	Study of Crust and Upper-Mantle Attenuation in Central and Northern California
HP-93-47	Mark Bukowski	UC Berkeley, Geology and Geophysics Dept.	David Boercker	Bonding in SiO ₂ : First-Principles Calculations for Several Crystalline Configurations
HP-93-48	David Benson	UC San Diego, Applied Mechanics and Engineering Dept.	Randy Christensen	The Computational Modeling of the Shock Compaction of Ceramics
HP-93-50	Jeff Wolfenstein	UC Irvine, Mechanical and Aerospace Engineering Dept.	Mark Beeman	High-Pressure Synthesis and Deformation of Alkali Halides
HP-93-52	H.-R. Wenk	UC Berkeley, Geology and Geophysics Dept.	William Durham	The Development of Anisotropy in Ice
HP-93-55	John Wasson	UC Los Angeles, IGPP	Andrew Gratz	Experimental Investigation of Shock Effects in Porous Meteoritic and Terrestrial Materials
HP-93-56	David Webb	UC Davis, Physics Dept.	C.-S. Yoo	Preparation and Characterization of Iron and Iron Alloy Thin Films on Diamond Substrates
HP-93-57	M. Brian Maple	UC San Diego, Physics Dept.	William Nellis	Shock Compaction of Ferromagnetic Nanoparticles
HP-93-58	Joanna McKittrick	UC San Diego, Applied Mechanics and Engineering Dept.	William Nellis	Shock Compaction of Nanocrystalline and Glassy Oxide Ceramics
HP-93-59	George Wolf	Arizona State University, Chemistry Dept.	Andrew Gratz	Raman and High-Resolution Electron Microscopy Studies of Shock Amorphization in Silica
HP-93-61	Raymond Jeanloz	UC Berkeley, Geology and Geophysics Dept.	Andrew Gratz	Shock Synthesis of Amorphous Fe ₂ SiO ₄

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