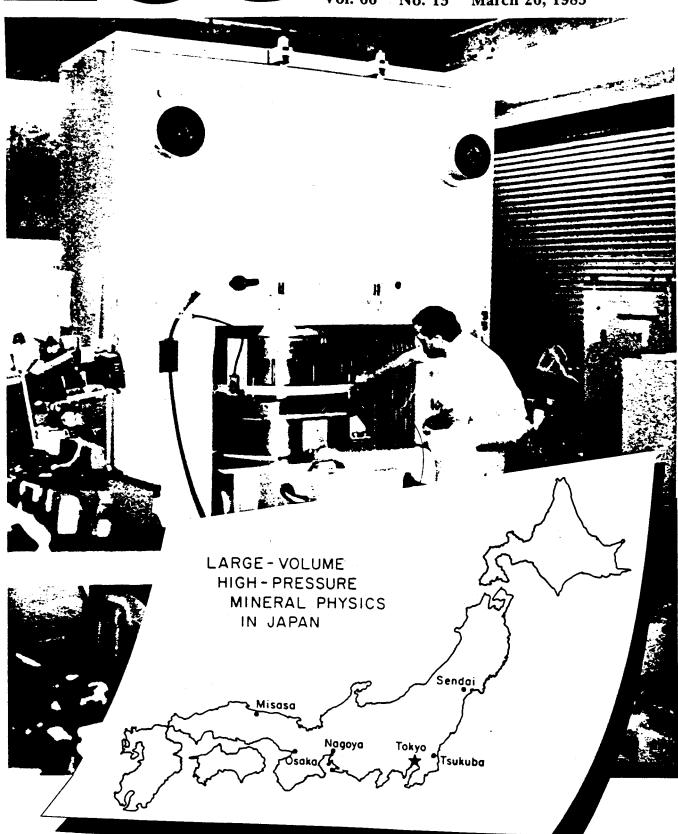
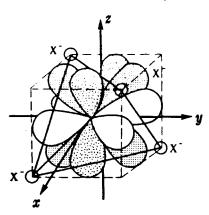
# EOS

Transactions, American Geophysical Union Vol. 66 No. 13 March 26, 1985



# Mineral Physics News



The focal point for the mineral physics community.

Editor: Robert M. Hazen, Carnegie Institution of Washington, Geophysical Laboratory, 2801 Upton Street, N.W., Washington, DC 20008 (telephone: 202-966-0334).

### Large-Volume High-Pressure Mineral Physics in Japan

Robert C. Liebermann, Charles T. Prewitt, and Donald J. Weidner

American high-pressure research with large sample volumes developed rapidly in the 1950's during the race to produce synthetic diamonds. At that time the piston cylinder, girdle (or belt), and tetrahedral anvil devices were invented. However, this development essentially stopped in the late 1950's, and while the diamond anvil cell has been used extensively in the United States with spectacular success for high-pressure experiments in small sample volumes, most of the significant technological advances in large-volume devices have taken place in Japan.

Cover. (top) The 5000-ton uniaxial press and split sphere apparatus in laboratory of E. Ito at the Institute for Study of the Earth's Interior of Okayama University in Misasa, Japan. Such large-volume presses provide an important source for synthetic mineral samples of phases thought to exist in the earth's mantle. Pressures of 25 GPa can be exerted on specimens of several cubic millimeters with 1100-ton axial load. Author Robert Liebermann provides the scale. (bottom) Map of Japan, showing location of major research centers for mineral physics. Map and photograph courtesy of Liebermann and colleagues Charles Prewitt and Donald Weidner; see their article. "Large-Volume High-Pressure Mineral Physics in Japan" in the Mineral Physics News, this issue.

Over the past 25 years, these technical advances have enabled a fourfold increase in pressure, with many important investigations of the chemical and physical properties of materials synthesized at high temperatures and pressures that cannot be duplicated with any apparatus currently available in the United States.

We got a first-hand look at this activity during the second U.S.-Japan seminar on high-pressure geophysics, convened at Hakone in January 1981 by Syun-iti Akimoto and Murli Manghnani, and also during the laboratory tour that followed. In the summer of 1984, we paid a return visit to Japan, where almost all of the state of the art equipment in this field is now manufactured, to visit university and government research laboratories and to discuss technical specifications with several companies. We report here our impressions of the visit.

Large-volume, high-pressure research in mineral physics has enjoyed a long and vigorous history in Japan, largely because of the activities and influence of the 1983 Bowie medallist Syun-iti Akimoto at the University of Tokyo, Mineo Kumazawa at Nagoya University, and the late Naoto Kawai at Osaka University. Much of the current excitement and vitality of mineral physics research in Japan is illustrated in papers contained in two recent books. High-Pressure Research in Geophysics [Akimoto and Manghnani, 1982] includes papers presented at Hakone in 1981. Materials Science and the Earth's Interior [Sunagawa, 1984] describes the results of a 3-year national program in Japan that was designed to bring together scientists from geophysics, mineralogy, petrology, and materials science for a coordinated attack on the properties and processes of the earth's interior (see also book review by Weidner [1985]). The intensity of the Japanese commitment to large-volume, high-pressure research was also made evident at a U.S.-Japan Seminar entitled "Partial Melting Phenomena in the Earth and Planetary Evolution," held in Eugene, Oregon, on August 31-September 7, 1984, convened by Harve Waff and Mineo Kumazawa; the proceedings of this seminar are to be published in the Journal of Geophysical Research in late

On our 1984 trip, we were struck by several aspects of current activity:

- The evolution of many of the high-pressure systems toward similar two-stage configurations for generating the highest pressures
- The extension to temperatures above 2000°C, simultaneous with very high pressures
- The growth of large single crystals for physical property measurements
- Experiments on more complex petrological assemblages
- The interfacing of such large-volume apparatus with a synchrotron X radiation source.

To improve alignment and to ensure synchronous application of force on the compressed volume, most multianvil devices are now confined in a pair of guide blocks

("buckets" in Figure 1) which are themselves driven by a uniaxial press (Figure 2 and cover photo). In the DIA apparatus (Figure 1a) developed by Kobe Steel, the anvil heads (ah) are made of tungsten carbide and compress a cubic sample assembly (S) oriented with its [100] axis vertical. As a consequence of this geometry, this apparatus is particular y wellsuited for in situ X ray diffraction measurements at high pressures. As with all the highpressure systems discussed here, there is a significant trade-off between the size of the sample assembly and the maximum pressure attainable. With anvil edge length of 6 mm, pressures of 10 GPa (100 kbar) can be obtained; if this length is reduced to 2 mm, the pressure limit increases to 20 GPa. Anvils can be interchanged easily between experiments.

The wedge apparatus (Figure 1b) invented by M. Wakatsuki is similar in principle to that developed at the National Bureau of Standards in 1959. As in the DIA apparatus, the anvil heads slide on the inside surface of the guide blocks and are electrically insulated from one another so that alignment is auto-

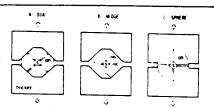


Fig. 1. A schematic illustration of various multiple anvil systems with upper and lower guide blocks ("buckets") driven together by uniaxial load (see arrows). Here ah is the anvil head and S is the cubic sample assembly to be compressed. Diagram from paper by M. Kumazawa and S. Endo in the volume by Sunagawa [1983].

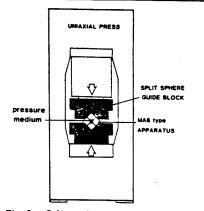


Fig. 2. Schematic illustration of large-volume high-pressure system with uniaxial press driving split sphere guide blocks. Six anvil heads cemented into guide block compress a cubic sample assembly (MA-8 type) that, in turn, compresses octahedral pressure medium (details in Figure 3). Diagram of system developed and installed by E. Ohtani in A. E. Ringwood's laboratory in Canberra, Australia.

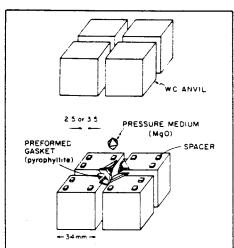


Fig. 3. MA-8-type cubic sample assembly developed by H. Sawamoto and M. Kumazawa in Nagoya University. An octahedral pressure medium is confined within an assembly of eight tungsten carbide cubes, each of which has been truncated on one corner to form a triangular face. This MA-8 assembly is then compressed isotropically by six larger anvils which are seated in a pair of guide blocks. Pressures of 25 GPa can be exerted on the pressure medium with triangular faces of 2.5 mm on the anvils and a 1000-ton axial load. Diagram from an unpublished work by H. Sawamoto.

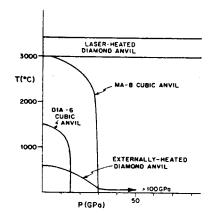


Fig. 4. Temperature-pressure range accessible with various types of high-pressure apparatus.

matically maintained during compression. and it is a simple matter to introduce signals into the specimen chamber. The cubic sample assembly S is oriented with the [111] axis vertical, which makes it less convenient for X ray experiments but quite suitable for synthesis experiments over a wide range of pressures from 2 GPa with 40 mm tungsten carbide anvils to 9 GPa with 10 mm anvils. The anvils are more massive in this device than in the DIA: thus they require a longer time to exchange and are quite expensive to replace if broken. The wedge apparatus is also often used in a two-stage configuration described below.

In the split sphere apparatus originally developed by Kawai, six anvil heads were enclosed in a heavy rubber spherical jacket and immersed in an oil pressure vessel. As now

used by Ito (Figure 1c), the anvil heads are permanently glued into a spherical seat in the steel guide block. This anchoring makes it more difficult to guarantee continuous alignment but also reduces the stress concentration in the buckets so that smaller buckets can sustain the same uniaxial force as that in the DIA or wedge apparatus. As a consequence of the fixed position of the tool steel heads, the split sphere apparatus operates only in the two-stage configuration described below.

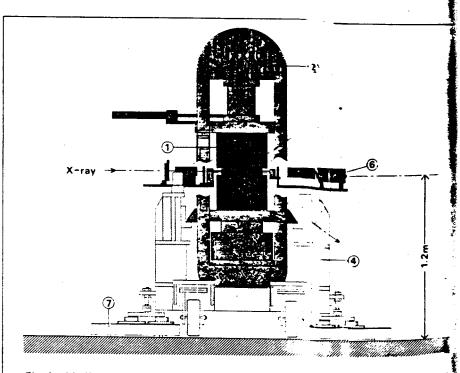
The highest pressures are obtained when these cubic anvil systems are operated in two stages, which are illustrated in Figure 3 for the system developed at Nagoya by Kumazawa and Sawamoto. An octahedral sample assembly is contained inside a set of eight tungsten carbide anvil cubes, each of which has one corner truncated into a triangular face. These eight anvils collectively form a second-stage cubic sample assembly (called the MA-8 system) which is, in turn, compressed by the six anvils of the first stage of either the wedge (Figure 1b) or split sphere apparatus (Figure 1c). Then the principle of cascading compression allows higher pressures to be achieved inside the second stage of compression. These two-stage configurations are now being used to generate pressures in excess of 25 GPa for octahedral sample assemblies with edge lengths of 2 mm, which can incorporate specimen charges of several cubic millimeters. The range of accessible pressures and temperatures for these devices is illustrated in Figure 4 and compared to the range for the externally or laserheated diamond anvil cell.

The uniaxial presses necessary to drive these high-pressure, large-volume devices come in a variety of shapes and sizes. The DIA-6 is operated with a two-post press capa-



Fig. 5. 2.0 wm press and DIA-6 apparatus in additionary of S. Akimoto at the Institute to Nobel State Physics of the University of Yokyo. A rotating anodetype high-senset X ray source used for issue X ray little tion measurements is alseen in Protect the DIA-6 apparatus. Scale council of T. Yagi (now at Tohoke University in Neudai).

ble of 250 tare of axial force (Figure 5). The wedge and regard devices are driven by four-post hy frame presses of 700- and 200 ton capacity as Maximely. The large split sphere system shown in the cover photo is contained wature a laminated picture frame



for in situ X ray diffraction experiments with the synchrotron radiation source at the Photon Factory of the National Laboratory for High-Energy Physics in Tsukuba, Diagram from a paper by Shimomura et al. in the volume by Minomura 1985.

type press capable of a 5000-ton load, although experiments at sample pressures of 25 GPa now require only a 1100-ton load.

The focal point of high-pressure research in Tokyo has been Akimoto's laboratory at the Institute of Solid State Physics. Their first large-volume apparatus was the tetrahedral anvil press (see cover of Eos, July 5, 1983) which is still used for synthesis of starting materials up to 8 GPa. Current research in this field is concentrated on the use of a DIA-6 apparatus (Figure 5) to study the dissolution of hydrogen in iron at high pressure and the resulting implications for the composition of the earth's core. Experiments with the wedge apparatus in a single-stage configuration include the growth of large single crystals of black phosphorous from a melt and of Ni2SiO4 spinel via a solid-solid phase transformation. Phase equilibria studies on CdGeO3 in the two-stage configuration have revealed that this compound undergoes successive phase transformations from pyroxenoid to garnet to ilmenite to perovskite structures with increasing pressure. At pressures up to 17 GPa, large volumes of enstatite-pyrope garnet assemblages are being synthesized for calorimetric measurements in A. Navrotsky's laboratory in the United States.

in

lso

ku

he

400-

oom

In the Department of Earth Sciences at Nagova University, mineral physics research at high pressures has been developed under the leadership of M. Kumazawa, who recently has moved to the Geophysical Institute of the University of Tokyo and has been succeeded at Nagova by H. Sawamoto. Their equipment includes 17,000-ton and 2000-ton presses, both equipped with the Nagoya MA-8 highpressure device. In the adjoining Department of Engineering, there are DIA-6 and DIA-15 cubic anvil systems. An innovation by Sawamoto has made it possible to achieve, and sustain stably, temperatures of greater than 2000°C for periods of more than I hour. The conventional graphite heater is surrounded by a sleeve of LaCrO3 which is an insulator at low temperatures. As the cell temperature rises above about 1000°C at pressures above 10 GPa, the graphite converts directly to diamond, and the LaCrO3 begins to act as the heater. Temperatures of 2500°C have been generated, thus enabling the determination of melting curves for Mg2SiO4 and MgSiO3 to pressures of 25 GPa. Experiments at these extreme temperatures also necessitate changes in the pressure medium (Figure 3); above 1200°C and 10 GPa, pyrophyllite decomposes into a stishovite-bearing assemblage and has been replaced by semi-sintered MgO (porosity ~30%). These extreme temperatures at high pressure have also facilitated the growth of large single crystals of the beta and gamma spinel phases of Mg<sub>2</sub>SiO<sub>4</sub>; the elastic properties of these crystals have been determined by using Brillouin spectroscopy by Sawamoto and Weidner at Stony Brook.

In the small village of Misasa, a few kilometers inland from the Japan Sea, Okavama University operates the Institute for the Study of the Earth's Interior (formerly the Institute for Thermal Springs Research). The high-pressure laboratory is under the direction of E. Ito, who was a student of Kawai. The split sphere system that he now uses,

which has a 5000-ton press, has been described above (cover photo, Figures 1c and 2) and has been used to show that the phase boundaries between the ilmenite and perovskite phases of MgSiO3 and the spinel and periclase + perovskite phases of Mg<sub>2</sub>SiO<sub>4</sub> have negative Clapevron slopes dP/dT. Studies of the phase relations in the MgO-FeO-SiO<sub>2</sub> system at very high pressures have elucidated the partitioning of iron between the magnesiowüstite and perovskite phases into which olivine disproportionates above 20 GPa. Ito has also synthesized large quantities of powder and single crystal specimens and studied their thermochemical and elastic properties during an extended visit to the United States last year.

The development of these large-volume systems for ultra-high-pressure, ultra-hightemperature research has involved considerable technical skill, and early research has been focused primarily on simple mineralogical systems. Now that these systems have become more "user friendly." they have begun to attract increased attention from the experimental petrology community, whose horizons have heretofore been largely limited by the pressure range of the piston cylinder apparatus (≤5 GPa). The techniques and concepts of experimental petrologists are now being incorporated in experiments on garnet peridotite and chondrite compositions in both the Misasa and Nagova laboratories.

Tsukuba Academic New Town is Japan's "Science City." It is located about 60 km northeast of Tokyo and is the home of the

northeast of Tokyo and is the home of the University of Tsukuba and more than 40 government research institutes, as well as a growing number of laboratories and related facilities being built by private companies. Large-volume high-pressure research is an important component of activities at the National Institute for Researches in Inorganic Materials (NIRIM), the Materials Science Department at the University of Tsukuba, and the Photon Factory at the National Laboratory for High-Energy Physics. At NIRIM an extensive program for synthesis and research on a variety of materials is under the direction of O. Fukunaga. In particular, this group is interested in the synthesis of diamonds and other ultrahard materials and recently completed the construction of a 30,000-ton press (the largest of its kind in Japan and the largest anywhere, except for the 50,000-ton press in Moscow) for use with a belt-type apparatus and for the synthesis of large quantities of materials such as sintered diamond and cubic boron nitride. Other equipment at NIRIM includes a 14.000-ton press with belt-type anvils, a DIA-20 cubic anvil guide block and press, and several smaller

As indicated above, the DIA-type apparatus is ideally suited to in situ X ray diffraction-measurements of samples under simultaneous high pressure and high temperature. A team led by O. Shimonura of NIRIM and T. Yagi of Tohoku University (Sendai) has taken the lead in developing large-volume systems for use with synchrotron X radiation sources by designing and constructing a 500-ton uniaxial press equipped with a DIA-10 cubic anvil system for the 2.5-GeV storage ring at the

Photon Factory (Figure 6). Currently, this system is being operated on a bending magnet beam line in the energy dispersive mode with a solid state detector. However, it could be used with monochromatic radiation or on a port with a wiggler magnet that would produce much higher energy radiation for energy dispersive applications. Named the MAX-80 (for multianvil-type high-pressure X ray system designed in 1980), it can produce pressures up to 10 GPa in a volume 6 mm on an edge with simultaneous temperatures above 1000°C (note that diamond anvil cells are rarely operated above 600°C so as to prevent the diamonds from oxidizing or converting to graphite). One of the first applications of the MAX-80 was to observe the direct conversion of graphite to diamond. The ability to study kinetics of synthesis in real time will be extremely useful in optimizing the conditions for growth of new high-pressure phases. While in Japan, we also had the opportunity to observe a 1-day experiment using the MAX-80 to determine the olivine-spinel phase boundary in Fe<sub>2</sub>SiO<sub>4</sub> between 900° and 1500°C (including reversal of this boundary) using NaCl as an in situ pressure standard. Preliminary reports of the applications of the MAX-80 for high-pressure, high-temperature mineralogy appeared in the recent book edited by Minomura [1985].

At the University of Tsukuba, M. Wakatsuki operates a high-pressure laboratory containing the wedge apparatus that he developed with K. Ichinose when he worked at the Toshiba Corporation. Wakatsuki is well known for his work on diamond synthesis and on the relation of crystal size and morphology to synthesis conditions; he is continuing this work at Tsukuba.

Following our visit to Japan and the ensuing technical discussions, we are now entering the final planning phase for the development of such large-volume high-pressure facilities in our laboratory at Stony Brook. These will be the first such facilities in the United States, and we expect that many North American and overseas colleagues will visit the laboratory to collaborate in research once the new facilities become completely operational (the target date is mid-1986). We hope to describe these installations more fully in a subsequent issue of the Mineral Physics News.

### References

Akimoto, S., and M. H. Manghnani (Eds.). High-Pressure Research in Geophysics, Center for Academic Publication Japan. Tokyo. 1982.

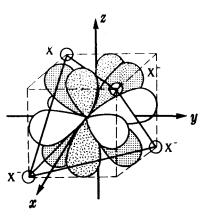
Minomura, S. (Ed.), Solid State Physics Under Pressure: Recent Advances With Anvil Devices, KTK Scientific, Tokyo, 1985.

Sunagawa, I. (Ed.), Materials Science and the Earth's Interior, Terra Scientific, Tokyo, 1984.

Weidner, D. J., The interior of the earth, Science, 227, 48, 1984.

Robert C. Liebermann, Charles T. Prewitt, and Donald J. Weidner are with the Department of Earth and Space Sciences, State University of New York, Stony Brook.

# Mineral Physics News



The focal point for the mineral physics community

Editor: Robert M. Hazen, Carnegie Institution of Washington, Geophysical Laboratory, 2801 Upton Street, N.W., Washington, DC 20008 (telephone: 202-966-0334).

### Rock and Mineral Physics at University College London

P. F. Dennis, P. G. Meredith, and G. D. Price

The Department of Geological Sciences at University College London (UCL), has undergone a period of major expansion and growth as a result of the restructuring of geology departments within the University of London that was carried out in 1982. This exercise produced the amalgamation of selected parts of the Department of Geological Sciences of Queen Mary College and the Department of Geology, UCL, on the UCL site. The creation of this strengthened grouping has been successful in attracting a significant number of active researchers in the field of rock and mineral physics (RMP) to the new UCL department. As a result, the academic staff has more than doubled since 1982 and now stands at 31. Of these, 11 work in RMP, including one research professor, five tenured staff, and five postdoctoral research associates. Nine postgraduate research students also work in the RMP group

Of specific interest to the RMP group at UCL are the mechanical and rheological properties of rocks and the nature of defects in crystals, with specific reference to their influence on the physical properties of minerals. Research in the group focuses on a series of problems, ranging from those dealing with the cover rocks of the crust and basin processes to the structure and bonding of mantle-forming phases and their influence upon mantle dynamics and plate motion. To investigate these problems, the group uses a variety of advanced experimental techniques, including high-pressure and temperature tri-

axial creep apparatus, acoustic emission monitoring of fracture propagation, holographic interferometry of deformed surfaces, and diffraction and microspectroscopic methods. These experimental investigations are coupled with computer modeling of physical processes at both the mesoscopic and atomic levels and are further supported by original theoretical studies and development. In this article, we review experimental capabilities and current research activities of the recently formed RMP team.

### **Crystal Physics**

The behavior and properties of high-density mantle-forming silicates and their influence on mantle dynamics and rheology are the major research interests of David Price. He combines experiments performed on analog materials with theoretical and computerbased techniques of molecular dynamics and static simulations to shed light upon the behavior of MgSiO<sub>3</sub>-perovskite. The analog studies involve deformation experiments on oxide perovskites (e.g., CaTiO<sub>3</sub>); the experiments are performed with the high-temperature single-crystal creep apparatus at UCL, coupled with transmission election microscopic observations. These experiments are helping to provide an understanding of oxide perovskites rheological properties, which are not currently well known. As an alternative to the direct study and measurement of the properties of silicate perovskites, samples of which are not adequate for most experiments, Price is using computer-based models to calculate the structural, defect, and lattice dynamical properties of MgSiO<sub>3</sub>. He has developed atomistic models of silicates in which phenomenologically determined, pairwise additive, interatomic potentials are used to describe the effective forces between atoms in mineral structures. Such models are being used to investigate and predict the properties of perfect crystals and to calculate their elastic and spectroscopic characteristics, as well as to calculate the energetics of defects and the activation energies and volumes for diffusion and to investigate ionic conductivity.

In addition to mantle studies, Price is concerned with the defects developed in iron-titanium oxides and is particularly interested in the structure and properties of C-Fe<sub>2</sub>O<sub>3</sub>, which he is studying by X ray, neutron, and Mössbauer techniques. In collaboration with Paul Dennis, he is involved with computer modeling of the nature of incommensurate (IC) structures in insulators and is specifically interested in establishing the nature of the IC ordered structure of mullite. His interest in the factors that determine crystal structures and his research into polytypism have led him to the study of zeolites, and he is currently collaborating with Judith Milledge and Monica Mendelssohn on a project aimed at direct methods of crystal structure determination from X ray powder data. In addition, improvements in diffraction methods under development by Mendelssohn and Milledge at UCL include computational techniques to improve the performance of search/match programs that are used for the identification of components of mineral solid solutions and for streamlining procedures to ensure optimum performance in diffraction experiments where anomalous dispersion effects are either desirable or unavoidable.

Milledge and Mendelssohn are also continuing their long-term investigations of the structure and properties of diamond to take advantage of recent advances in experimental

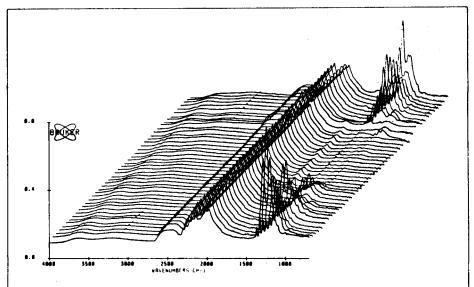


Fig. 1. A stack plot of the infrared spectrum across a natural diamond. The spectra were obtained by using a microscopic infrared beam (80-μ spot diameter) that was stepped at 100-μ intervals across the diameter of a diamond. Such micro-infrared studies are revealing hitherto unsuspected inhomogeneities and complexity in the defect chemistry of diamonds that more traditional, gross-scale studies are unable to detect. The potential for such microscopic spectroscopic studies, particularly when coupled with microanalytical techniques, is great and is being actively developed at UCL.

techniques. Diamonds commonly contain monocrystalline inclusions that are the best preserved specimens of mantle material known to us. Although such inclusions have long been the subject of diffraction and microprobe analyses, the host diamond itself was, until recently, mainly characterized by spectroscopic methods and then not on the submillimeter scale, at which significant variations can be revealed by X ray topography or chemical etching, even in apparently perfect gemstones.

New mass spectrometric techniques for establishing C and N isotope variations and nitrogen abundances in specimens of laser dissected diamond (on the order of 100 µg in weight) can now be correlated with infrared microspectroscopic measurements actually made on the same specimen (Figure 1). In a three-way collaboration between UCL, the Open University, and D. Drukker of Amsterdam, Mendelssohn and Milledge are planning to use artificial irradiation and heat treatment to simulate the effects of the pressure/temperature regime to which the diamonds, and hence their host rocks, have been subjected. Many diamonds are more than half the age of the earth and have suffered natural radiation damage severe enough to affect the nature and mobility of the defects that they contain. Cathodoluminescence, infrared spectroscopy, and X ray methods are used in studies of the nature and state of aggregation of the light elements (H, B, N, and O) that are present in almost all diamonds; and in collaboration with Carl O'Brien of the Statistical Sciences Department at UCL, these researchers have developed improved statistical techniques for the interpretation of multiple decay curves that are involved in topographic activation analysis experiments used to map trace element distributions in diamond and other minerals. In order to gain a better understanding of the mechanisms of isotopic fractionation, Milledge and Mendelssohn are using a Kossel camera with a custom-built liquid He stage in their scanning electron microscope to produce divergent beam diffraction patterns (Figure 2), to measure accurate lattice parameters of isotopically distinct specimens as a function of temperature, and hence to gain a better understanding of the behavior of isotopic solid solutions.

The major research interests of Paul Dennis are in the areas of the point defect chemistry and mass and electrical transport properties of minerals. As a complement to the computer modeling techniques used by David Price, he employs secondary ion mass spectrometry (SIMS) to trace stable isotope migration and thus to determine anion and cation self-diffusion coefficients. The data, determined over a range of conditions (T, P(O2), P(H<sub>2</sub>O), etc.) are used to model point defect chemistry and transport mechanisms in minerals. In addition to these kinetic studies, Dennis has developed and is using SIMS directly to measure equilibrium hydrogen contents in experimental samples. He is comparing the interpretation of results from this work with those of infrared spectroscopic

A major aim of the RMP group is to understand the dissolution mechanisms for water in nominally anhydrous silicates and in what ways these water-based defects may affect diffusion controlled processes. This research represents the first step in developing a valid micromechanistic model for hydrolytic weakening of silicates. Most of the experimental work has been based on quartz and the feldspar group minerals but is now being extended to include forsterite and other olivines.

In addition to these silicate studies, Dennis is also working on several oxide phases. In collaboration with David Price, he is looking at the diffusion kinetics in several oxide perovskites. The data, together with the results from rheological, electron microscopic, and computer simulation studies are important in understanding the high-temperature creep properties of mantle phase minerals. He is also studying several grossly nonstoichiometric oxides (e.g., TiO2) to help understand both the role of hydrogen in their defect structure and the effect of extended defects (e.g., crystallographic shears) on their diffusion behavior. At present, little is known about the role of extended defects in the behavior of possible mantle minerals (magnesiowüstite).

This combination of experimental diffusion measurements, computer simulation of defects, and spectroscopy at UCL provides a powerful approach to understanding physical properties of minerals.

### **Rock Physics**

Experimental and theoretical rock and ice deformation and thermomechanical modeling of tectonic and metamorphic processes in the crust and lithosphere are the major research interests of Stanley Murrell. He has recently designed and constructed a low-temperature servo-controlled triaxial apparatus (Figure 3) that is being used to study brittle cracking and creep deformation in both natural sea ice and laboratory-grown ice. The apparatus operates at pressures to 300 MPa (3 kbar) and temperatures to -100°C. This research is applicable not only to several areas of basic science of the earth and planets but also to engineering in arctic regions.

The laboratory also operates a high-temperature triaxial apparatus, pressurized by a 1400-MPa Harwood gas pump, which can now be used for experiments on rocks at temperatures exceeding 800°C, at which temperatures iron jackets and alumina pistons are used. In addition, acoustic velocity measurements can be made in this vessel to monitor crack-related deformation. The apparatus is currently being used to study both the deformation of mantle minerals and rocks and the brittle/ductile transition in rocks (especially silicates) under conditions typical of the lower continental crust. Of particular interest are the deformation properties where metamorphism (e. g. metamorphic dehydration or polymorphic phase changes) or partial melting occurs. Particular attention is paid to the relationship between single-crystal and polycrystalline deformation. Murrell's previous studies on creep extended to temperatures of 1200°C and was restricted to polycrystalline rocks. That work demonstrated the overlapping of several different rheological phenomena in polyphase rocks at high temperatures, namely brittle cracking, crystal plasticity, and partial melting. He is now extending his experiments to 1700°C and is studying single crystals and monomineralic polycrystals. From these experiments, he expects to ob-

serve valuable analogies between ice deforma-

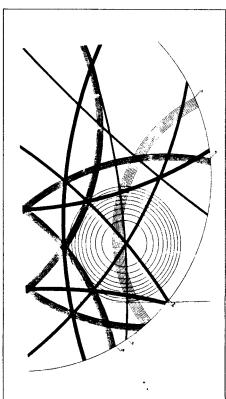


Fig. 2. Part of a set of "nested" conics from a computer simulation of a divergent beam image of LiF, produced by using  $\text{CuK}_{\alpha}$  radiation. The cell parameters used in this simulation range from 4.01 to 4.05 Å in steps of 0.0005 Å. The extreme sensitivity of position of some of these conics to cell parameters enables the technique to measure cell parameters extremely accurately, thus providing an opportunity for making detailed studies of the thermal expansion behavior of materials, the effect of isotopic substitution on cell size, and other subtle phenomena.

tion near 0°C and monomineralic rock deformation near the solidus.

Investigation of the fracture properties of rocks and minerals and their application to a wide range of problems of crustal rupture are the main research interests of Barry Atkinson and Philip Meredith. They are applying fracture mechanics and related analyses in order to better understand both fast (catastrophic) and slow (subcritical) crack growth in geological materials. This approach is preferred to a purely phenomenological one because it relates directly to the fundamental physicochemical processes and energetics involved. Of particular interest is the stable subcritical propagation of cracks enhanced by the chemical influence of environmental fluids ("stress corrosion"), which can allow crack growth to occur at stresses that can be much lower than the short-term fracture stress of the material and at crack velocities many orders of magnitude lower than those associated with catastrophic failure.

Much of their recent research effort has been expended in the experimental study and characterization of stress and corrosion enhanced subcritical cracking in a range of important crustal rock types and rock-forming minerals, with particular emphasis on the influence of temperature and activity of environmental species. In addition to these direct experimental measurements of fracture mechanics parameters, they are using a range of complementary techniques to monitor crack growth as deformation proceeds. The most important of these are acoustic emission monitoring and holographic interferometry. Current experimental developments center on the study of inelastic processes in rock fracture, with special reference to the characteristics of the microfracture process zone and its dependence on microstructure, deformation rate, and environmental conditions. In addition to these fracture mechanics studies. Atkinson and Meredith are investigating the high-pressure/high-temperature mechanical properties of rocks, particularly crack healing and strength recovery during low-cycle fatigue experiments under simulated crustal conditions.

The data from these studies are rapidly finding application in many important areas of current geological interest, such as earthquake rupture, energy production related technology, and failure prediction. Atkinson is particularly interested in rock mechanics constraints on earthquake source physics, especially the development of stress-induced crack anisotropy in earthquake preparation zones and its influence on seismic wave polarization and attenuation. In collaboration with Ian Main of the University of Reading (Reading, U.K.), Meredith is investigating geometric scaling laws in rock fracture to seek analogies between the distribution of acoustic emissions from laboratory specimens and earthquake magnitude/frequency distributions.

### Crustal Physics

Rock deformation studies in the department are also directed toward understanding the behavior of porous water- or hydrocarbon-saturated sediments. Mervyn Jones and Robert Preston are currently studying the behavior of these materials. Their investigations include the formulation of mathematical descriptions of sediment behavior through the combination of elasticity theory and critical state theory, experimental studies of sediment compaction, analysis of stress paths in natural sediment deformation, and the formation of fold and fault structures in sedi-

The leadership of the Department of Geological Sciences at UCL in sediment deformation studies has been achieved through the development of a highly advanced triaxial testing system. This apparatus permits deformation at elevated temperatures (up to 200°C) and pressures (up to 70 MPa) to be modeled along any one of a number of stress paths. Axial and radial deformation of specimens can be controlled to within 1.5 µm (the original specimen size is 76 mm long by 38 mm in diameter), and the volumetric strain can be independently determined. The pore fluid pressure can be maintained at any pressure up to 70 MPa during drained tests and up to the axial stress (200 MPa) during undrained tests. In addition to this high-pressure triaxial cell with stress path capability, an odometer with a similar operating range is also employed in the laboratory.

This equipment is now providing Jones and Preston with significant new data that indicate that the mechanical behavior and com-

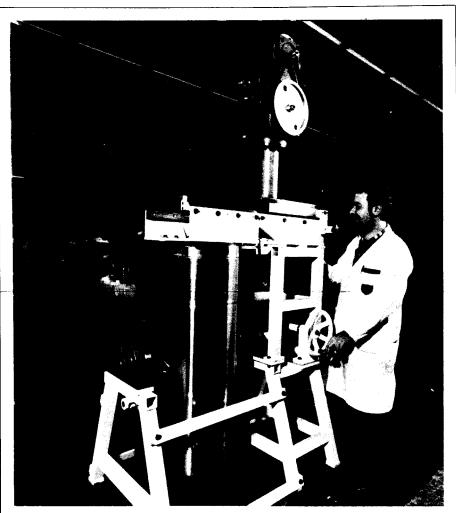


Fig. 3. The low-temperature high-pressure triaxial compression testing cell for ice deformation was developed as the result of a collaborative project between UCL and British Petroleum. This apparatus, normally housed in a cold room, can deform 100 mm long by 40 mm in diameter ice samples at temperatures down to -100°C and at confining pressures up to 300 MPa, utilizing a 100-kN servocontrolled actuator. It is currently being used in a study of the rheological behavior of sea ice, but studies of pure water ice are also planned.

paction of porous sediments are best described by a modified consolidation equation and critical state theory. Failure is thus defined both in terms of the onset of volumetric deformation (elastic limit) and the onset of constant volume shear deformation (critical state limit). The compressibility of the sediment is defined by a stress window in effective stress path space between these two limits and, once defined, may be used in reservoir engineering studies to predict oil field subsidence and compaction driving and in geological studies to back-analyze the volumetric strains associated with sediment deformation and burial. Conversely, naturally occurring textures may be used to identify this stress window for some sediments, although such paleostress analyses are still in their infancy. This approach to sediment deformation is both new and exciting; in addition, it provides far greater insights into sediment behavior than the traditional rock mechanics studies, which are more appropriately confined to thoroughly lithified materials.

Other studies now being conducted within the department couple the principles of classical mechanics with rock mechanics data that relate to elasticity, brittle fracture, and other physical parameters. These studies are leading to interpretation of the deformation of rock masses, which may be treated as either continuous or discontinuous media. Applications range from qualitative analyses of deformation of the lithosphere to quantitative analyses of specific structures and situations related to cover rock deformation. Consequently, these studies form an important linking element between rock deformation studies conducted in the laboratory and more traditional geological field studies.

The mechanics of lithospheric deformation, with special reference to a specific region in the East Indies archipelago and its control of the geological evolution of the area, is being studied by Michael Audley-Charles and Neville Price. The model is qualitative but is proving to be a powerful tool in predicting details of regional evolution. Wherever pertinent geological information is available, the correlation between predicted and observed behavior is excellent. Although it is designed to explain the geological evolution of a relatively restricted area, the model is providing insight into the evolution of a

much wider area of the East Indies and is likely to have application in many other localities in the world.

Quantitative analyses of cover rock deformation, with special reference to the development of fractures, high fluid pressures, and fluid migration in basins, are also being conducted by Price. At this early stage in the investigation, a modular approach is being used. For example, a study of the stress and fluid pressure development in a hypothetical half graben yields specific conclusions regarding the form and evolution of "rollover" structures of complex geometry and the generation of "tectonic inversion." These conclusions, however, are pertinent to other geological environments. In particular, the analysis points to the essential importance and interlinking of deformation and fluid pressure: high fluid pressure promotes deformation, which in turn enhances the development of even higher fluid pressures.

### The Future

In the future, the members of the RMP group at UCL hope to develop their special combination of skills and expertise to tackle major interdisciplinary problems. Of particular interest are ways in which we can use our detailed understanding of mineral physics to interpret and explain the behavior of rocks as polycrystalline aggregates (under crustal and mantle conditions). Such an understanding will require a significant research effort into the effect of interfaces and grain boundaries upon the physical responses and behavior of materials. Similarly, we hope to use our detailed understanding of the behavior of rocks and sediments to model and mechanistically interpret large-scale geological processes ranging from earthquake rupture to mantle dynamics.

The RMP group at UCL welcomes communication and visits from any other scientists who have interests in rock and mineral physics research. For further information, contact the authors, P. F. Dennis, P. G. Meredith, and G. D. Price, at the Department of Geological Sciences, University College London, Gower Street, London WC1E 6BT, U.K.

Paul Dennis, Philip Meredith, and David Price are all with the Department of Geological Sciences, University College London.

# News & Announcements

### Mineral Physics News Briefs

### Peridotite Melting at High Pressure

Melting experiments on peridotite are crucial to our understanding of magmatic origins because these olivine-pyroxene rocks are believed to form most of the earth's upper mantle. In a report published in *Nature* (vol. 315, 566–568, 1985), E. Takahashi and C. M. Scarfe describe peridotite melting experiments at pressures to 140 kbar that were performed in the large-volume, split sphere apparatus at Okayama University, Misasa, Japan

(see Eos, March 26, 1985, p. 183). These experiments greatly extend the range of known melting relations for this rock type. Previous investigators have found that initial melts are basaltic in composition when generated from peridotite at melting pressures of 30-40 kbar. The new data of Takahashi and Scarfe reveal that, in contrast, at 50-70 kbar the initial melts are magnesium-rich and komatiitic in composition.

Considerable debate has occurred regarding the origins of komatiites, which are eruptive rocks with 24%-32% MgO and which are found almost exclusively in terrains of Archean age. Some researchers maintain that they arose from high degrees of melting (more than 50%) of mantle peridotite, whereas others suggest that komatiites were derived from initial melting and thus represent eutectic compositions. From the new experimental data the authors infer that komatiite genesis occured by low degrees of partial melting at 150-200 km depth in the Archean upper mantle

### New Data on Stishovite Lattice Vibrations

Stishovite, a high-pressure phase of SiO<sub>2</sub> with the tetragonal rutile-type structure, has been the subject of much mineral physics research. An unsolved dilemma with this phase has been the apparent lack of correspondence between stishovite's tetragonal symmetry, as deduced by X ray diffraction studies, and its vibrational spectra, which have appeared to be more complex. Russell Hemley, Ho-Kwang Mao, Peter M. Bell, and S.-I. Akimoto, in experiments to be published in Physica, have employed a micro-optical spectrometer at the Geophysical Laboratory of the Carnegie Institution of Washington, D.C., to obtain high-resolution Raman spectra of pure, synthetic stishovite for the first time. Bands at 231, 589, 753, and 967 cm<sup>-1</sup> are resolved and are assigned as the  $B_{1g}$ ,  $E_g$ ,  $A_{1g}$ , and  $B_{2g}$  fundamentals, respectively, of the first-order spectrum. Thus the character of the spectrum for synthetic stishovite is consistent with the ideal, ordered rutile structure. It is possible that some natural stishovites, such as the material from Meteor Crater employed in previous spectroscopic studies, may suffer from impurities, structural disorder, or defects induced by its shock

### Theoretical Modeling of Silicates at Pressure

A number of computational quantum techniques are now being applied to predict the behavior of solids at high pressure. Recent advances in one of these procedures, the modified electron gas (MEG) method, have led to predictions of the equations of state, lattice dynamics, and stability of oxide and silicate phases of interest to geophysicists. Until recently most of these computations have been applied to simple oxides, such as MgO and CaO. Thus a significant development is a series of publications that apply MEG methods to the silicate perovskites, now thought to be major mineralogical components of the deep mantle. These phases, such as MgSiO3, have proved very difficult to study in the laboratory because they can be synthesized in only small amounts and in some cases are nonquenchable.

Workers at the University of California at Berkeley, including M. S. T. Bukowinski, R. Jeanloz, and G. H. Wolf, have been able to rationalize the observed orthorhombic distortions from the ideal cubic structure of MgSiO3 in terms of instabilities found in a lattice dynamics calculation (Geophysical Research Letters, vol. 12, 413-416, 1985). By using a refined MEG model, R. J. Hemley (Geophysical Laboratory of the Carnegie Institution of Washington, D.C.) and M. D. Jackson and R. G. Gordon (Harvard University, Cambridge, Mass.) calculated the lattice parameters of the distorted MgSiO<sub>3</sub> perovskite structure and reproduced observed values to within 2% (Eos, April 30, 1985, p. 357 (abstract)). Furthermore, they found that the orthorhombic distorted phase should persist to very high pressures that are characteristic of the earth's lower mantle.

### **Editor's Note**

Brief summaries of significant new experimental or theoretical results of interest to the mineral physics community are welcome. Please send information to the Mineral Physics News Editor.

### Meetings

### U.S.-Japan High-Pressure Meeting

On January 13-17, 1986, there will be a conference entitled "High-Pressure Research and Applications in Geophysics and Geochemistry" in Kahuku, Hawaii. This joint U.S.-Japan meeting, the third in the series sponsored by the U.S. National Science Foundation and the Japan Society for the Promotion of Science, will bring together approximately 40 scientists engaged in studies related to geophysics and geochemistry of the earth's interior so that they may discuss many stateof-the-art techniques in laboratory experiments and theoretical calculations. Principal topics will include high-pressure applications of synchrotron radiation, light scattering and optical spectroscopy at high pressure, chemistry and physics of the earth's deep interior, bulk chemistry and differentiation in the mantle, and new techniques and synthesis of materials. For additional information, contact M. Manghnani, Hawaii Institute for Geophysics, 2525 Correa Road, Honolulu, HI 96822.

### International Mineralogical Association

On July 13–18, 1986, the 14th General Meeting of the International Mineralogical Association (IMA) will be held in Stanford, Calif. Several symposia at the IMA meeting will be of special interest to the mineral physics community. These sessions include mineralogical applications of synchrotron radiation, structural classification of minerals; thermodynamics and kinetics of mineral reactions; ordering, transformations, and modulated structures in phyllosilicates; structural and magnetic phase transitions of minerals; physics and chemistry of mantle minerals; applica-

tions of solid-state NMR to minerals; defect structures in minerals; and electron microscopy of the kinetics of mineral transformations. In addition, symposia will focus on specific mineral groups, petrology of igneous rocks, optical microscopy, industrial mineralogy, and other topics. Plenary lectures by Ekhard Salje on the application of order parameter theory to the thermodynamic properties of phase transitions and by Ian Jackson on the elasticity of mantle minerals will also be of special interest to mineral physicists. For additional information on the IMA meeting, write to IMA 1986, Department of Geology, Stanford University, Stanford, CA 94305.

# Quantum Theory and Experiment

On July 21-26, 1986, a conference entitled "Quantum Theory and Experiment Applied to Solids," will be held in College Park, Md. This conference will bring together theoreticians and experimentalists from the fields of mineralogy, geophysics, solid state physics, and chemistry. Its objectives are first, to examine the capability of various theoretical methods, including solid state band theory, ionic model simulation, molecular cluster theory, and qualitative MO band theory for explaining the properties of solids; second, to present recent experimental data on solids at extreme pressure and temperature, defect solids, glasses and surfaces to which the above methods may be applied, and third, to focus on some particular topics of current and future interest to mineralogists and other solid state scientists. For more information, contact the organizers, Jack Tossell (Department of Chemistry, University of Maryland, College Park, MD 20742) or G. V. Gibbs (Department of Geological Sciences, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061).

### Chairman's Corner

# Mineral Physics: New Choices and Directions

The Mineral Physics Committee convened a workshop October 16–18, 1985, at Lake Arrowhead, Calif., to examine the new directions in mineral physics for the next 5 years. The proceedings of this workshop will provide an explanation to the geophysical and geochemical community of the great new opportunities available to mineral physicists to bear on some of the outstanding problems of the earth. These proceedings will be published within a few months.

The Mineral Physics Committee is at a critical turning point. It became evident at the workshop that a number of new advances will soon provide dramatic advances in our understanding of the earth. Two of them will be mentioned here.

It is now clear that experiments on artificially produced minerals can be done in situ; that is, properties can be measured at the pressures and temperatures at which the mineral is stable. Three trends are bringing this about:

• Synchrotron radiation methods are beginning to replace classical X ray methods so that the experiment is over quickly.

• More artificially produced minerals are being synthesized so that our sample pool is increasing.

• Experiments are being perfected for application to smaller and smaller samples.

The day is coming when mineral physicists will determine, as experimental fact, how an assemblage of minerals change their phases into a different assemblage of minerals at selected conditions of the earth's upper mantle and perhaps even the top of the lower mantle.

A second trend is the increasing success of theoreticians in explaining the physical properties of minerals using fundamental principles. Accurate predictions of phase transitions, vibrational motion, structural variations, and physical properties like density and bulk modulus are now found in mineral physics sessions at every AGU meeting. There is even hope that theoreticians can address the time-dependent problems inherent in reaction mechanisms.

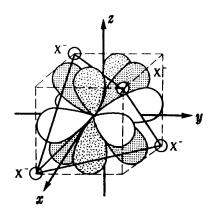
In some problems the mineral physicists have reached further than the seismologists. One example is their progress on the properties of iron. The density and sound velocity of iron at the earth's inner core conditions are known to a precision as good as, or perhaps better than, the seismically determined density of the inner core. By solving the phase diagram, mineral physicists have come to a good estimate of the temperature of the earth's core—near 6000°K—without recourse to seismically determined data.

Mineral physics seeks to understand how the physical and chemical properties of minerals control their geological and geophysical behavior, especially at high pressures and temperatures. Objectives of mineral physics include understanding properties of minerals on an atomic scale and using them to constrain the interpretation of global processes. Mineral physics provides the essential link between what we observe (e.g., seismic profiles) and what we would like to know (e.g., composition, temperature, and dynamics).

Mineral physics will always be a lively part of AGU as long as new techniques and new scientists come to its ranks from the sister disciplines of physics, chemistry, and mathematics. That is happening today. It is especially heartening to see young theoreticians trained in physics and chemistry presenting papers in AGU's meetings and journals—research that solves some outstanding problems in mineral ogy. In many cases, they are able to predict the phase changes and the physical properties of minerals that are at the limits of research by experimentalists.

Orson L. Anderson Chairman, AGU Mineral Physics Committee

# Mineral Physics News



Mineral Physics News:

The focal point for the mineral physics community.

Editor: Robert M. Hazen, Carnegie Institution of Washington, Geophysical Laboratory, 2801 Upton Street, N.W., Washington, D.C. 20008 (telephone: 202-966-0334).

### Mineral Physics and Mineral Chemistry at the Australian National University

Ian Jackson

Research at the Australian National University (ANU) in Canberra into the physics and chemistry of minerals is being actively carried out by a number of different research groups within the Research School of Earth Sciences (RSES), the Research School of Chemistry (RSC), and the Department of Geology. The research schools form part of the Institute of Advanced Studies, which is a national center for research and postgraduate training established by the Australian Government in 1946. The Institute of Advanced Studies seeks to ensure flexibility in its approach to research by maintaining an unusually high ratio (>1) of nontenured to tenured staff. Two types of nontenured appointment are available: postdoctoral fellowships of 1-2 yr duration and research fellowships tenable for 3-5 yr. The Department of Geology, as part of the Faculty of Science, is responsible for the provision of undergraduate education in geology, in addition to its role in research and postgraduate training.

A recent development aimed at fostering closer collaboration among the various mineralogy-oriented research groups on campus is the formation of an umbrella organization known as the Mineralogy Research Centre. The center also provides a forum for cooperation in staffing and in the provision of equipment, as exemplified by the creation of a joint appointment between RSES and RSC

for researcher Alex McLaren and the joint purchase of a Philips 300-kV Model 430 electron microscope with an extensive range of analytical attachments.

The personnel most actively involved in research into mineral physics and chemistry at ANU are members of the Petrochemistry Group (the current academic/research staff are Ted Ringwood, Lin-gun Liu, Hugh O'Neill, Tetsuo Irifune, Sue Kesson, and Nick Ware) and the Petrophysics Group (Mervyn Paterson, Alex McLaren, Ian Jackson, Steve Cox, and John Fitz Gerald) of RSES, the Solid-State Chemistry Group in RSC (Bruce Hyde, Alex McLaren, John Thompson, and Ray Withers) and Tony Eggleton's mineralogy-crystallography group within the Geology Department.

Current research that can be readily labelled mineral physics or mineral chemistry in the broadest sense falls into three main categories, which will be discussed below.

# Crystallography and Crystal Chemistry

The underlying theme of much of the work conducted by the Solid-State Chemistry Group is the search for a systematic and useful description of crystal structures based on an understanding of the factors that determine their stability. Recent studies by B. G. Hyde and Michael O'Keeffe (of Arizona State University, Tempe) have emphasized the influence of cation-cation interactions upon the stability and physical properties of certain crystal structures, some of which (e.g., quartz, olivine, spinel, diamond) are of major mineralogical significance.

Mechanisms of structural change are also being actively researched in a variety of contexts; for example, the spinelloids are being investigated because of their relevance to the mechanism of the olivine-spinel transformation (see Figure 1). Complex structures are also examined experimentally, e.g., sulphosalts such as cannizzanite, cylindrite, etc., and "modulated" versions of simple structures, such as  $\beta$ - $K_2SO_4$ -related types. Tony Eggleton and his colleagues are investigating the mechanisms of mineral hydration and oxidation, mainly in silicate weathering reactions, and the processes of clay mineral formation in hydrothermal alteration. The coordination of the nonsilicon cations in the parent mineral is found to exert a major control on the reaction process. Much of this work is dependent upon electron diffraction and high-resolution and analytical electron microscopy.

The continuing crystallographic problem of cation ordering in structural sites is being reassessed on a scale of nanometers by using convergent beam electron diffraction and channelled electron-enhanced X ray emission studies, especially of Al-Si ordering, symmetry, and modulation in framework silicates.

### Studies of Phase Equilibria

Much of the effort of the Petrochemistry Group in RSES continues to be devoted to the study of pressure-induced phase transformations and their bearing on the constitution

and dynamics of the earth's mantle. Laserheated diamond anvil apparatus is currently being used in studies of the stability of dense hydrated magnesium silicates. The installation of an MA8 multiple-anvil apparatus has paved the way for more thorough and systematic study of high-pressure phase equilibria than has been previously possible with laser-heated diamond-anvil apparatus. Early applications have been in the study of the melting of mantle minerals and in documenting the ultrahigh-pressure phase behavior for basaltic compositions. In the latter connection it has been conclusively demonstrated that subducted oceanic crust remains more dense than adjacent mantle and underlying lithosphere to depths of at least 600 km in the transition zone of the earth's mantle (Figure

Other major experimental studies of phase equilibria conducted in more conventional large-volume high-pressure apparatus have included investigation of the influence of pressure and temperature on the solubility of oxygen in molten iron and studies of the partitioning of elements such as Co and Ni between coexisting silicate and metal phases. Both of these studies bear directly on questions of the composition and formation of the earth's core and on the origin of the moon. Precise electrochemical measurements of the chemical potential of oxygen defined by certain key redox reactions, especially those associated with the quartz-olivine-metal buffers in the Fe, Ni, and Co silicate systems, are providing the thermodynamic framework within which silicate/metal partitioning and broader issues, such as the oxygen fugacity of the mantle (and its significance), can be dis-

## Mechanical Properties of Minerals and Rocks

The preoccupation of the Petrophysics Group (RSES) is the study of a wide spectrum of mechanical properties (elastic, anelastic, and plastic) of minerals and rocks. An integral part of such studies is the need for careful characterization of microstructures to gather evidence about processes that are induced in the laboratory and to help place the results in proper perspective in relation to natural rock and mineral systems.

Developments of improved procedures of ultrasonic interferometry allow for the accurate determination of the pressure dependence of the elastic moduli for single crystals and fine-grained polycrystalline aggregates of mantle minerals. A recent example is work on single-crystal wüstite  $Fe_{1p-x}O$ , which reveals a normal pressure dependence of  $C_{11}$  and  $C_{12}$  (and hence of the bulk modulus K) but a negative pressure coefficient for the shear modulus  $C_{44}$  that is the result of magnetoelastic interactions.

Increasing effort is being devoted to the experimental determination of shear wave velocities and attenuation at seismic frequencies by the observation and measurement of forced torsional oscillations. It has been found that for most rocks, the shear modulus

G increases rapidly with increasing pressure to  $\sim 100$  MPa at room temperature as a consequence of the closure of relatively low aspect ratio intergranular cracks (Figure 3). A corresponding decrease in the internal friction  $Q^{-1}$  is also observed.

A unique facility developed over many years by Mervyn Paterson and his colleagues provides for the study of the high-temperature rheology of rocks under a wide variety of experimental conditions by using gas medium apparatus. The weakening of minerals and rocks deformed in the presence of a hydrous fluid phase continues to be a focus for much of the experimental work. Particular attention is being paid to investigation of the solubility and diffusivity of water-related species in quartz and olivine. In a parallel development, pore-pressure effects and dilatancy in the ductile deformation of rocks are being explored.

Examination of microstructural features, such as H<sub>2</sub>O-related defect clusters in quartz, and dislocations, microfractures, and grain boundaries in various materials have provided important clues for identifying the processes associated with the experimentally observed mechanical properties. A highlight of recent work in the ductile field is the documentation by Shun-Ichiro Karato, Paterson, and Fitz Gerald of the transition between dislocation and diffusion creep in synthetic olivine aggregates (Figure 4). Extrapolation to natural conditions suggests that either (or both) of these mechanisms might be responsible for mantle deformation.

Ian Jackson of the Australian National University, Canberra, is a Foreign Correspondent of the AGU Mineral Physics Committee.

# News & Announcements

### High Pressure Experiments at 5.5 Mbar

The range of laboratory experimentation has been extended recently to pressures of 5.5 Mbar (0.55 TPa) in diamond anvil studies by J. A. Xu, H.-K. Mao, and P. M. Bell at the Geophysical Laboratory of the Carnegie Institution of Washington. This pressure range encompasses the entire earth from surface to core (central core pressures are estimated to be 3.5 Mbar), as well as pressures equivalent to the upper mantles of the giant planets. This enhanced ability to synthesize mineral phases, measure their properties, and observe their behavior will result in improved evaluation of models of earth and planetary interiors.

The high-pressure experiments to 5.5 Mbar involved implementation of new design concepts for the diamond anvil apparatus. In a previous experiment the maximum pressure achieved was approximately 2.8 Mbar, but the pressure calibration had to be done indirectly from load calculations. The shift of the fluorescent line of ruby crystals placed in the sample, which is normally employed as an internal pressure standard, could not be used in the earlier experiment because of strong interference from diamond anvil fluorescence at pressures above 2.7 Mbar. In the new experiments the overlapping diamond emission

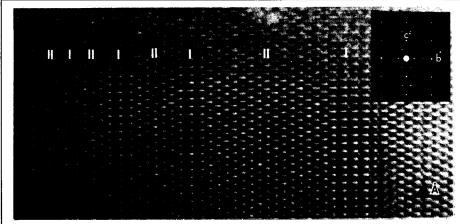


Fig. 1. [100] zone image of an intergrowth of phase I and II (major phase) in the NiAl<sub>2</sub>O<sub>4</sub>-Ni<sub>2</sub>SiO<sub>4</sub> system, observed in a sample quenched from 1400°C at atmospheric pressure (Hyde and colleagues at ANU).

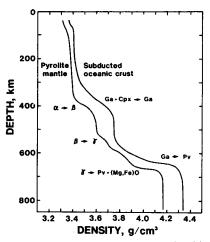


Fig. 2. Relative zero-pressure densities of subducted oceanic crust and adjacent mantle as functions of depth. The phase transformations responsible for most of the increase in density are indicated (Irifune and Ringwood).

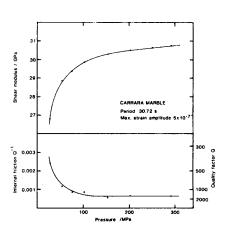


Fig. 3. The pressure dependence of the shear modulus and internal friction for Carrara marble at a period of 30 s and a maximum strain amplitude of  $5 \times 10^{-7}$  (Jackson and Paterson).

was found to disappear at pressures above 3 Mbar, and the ruby pressure calibration scale could be employed once again. The apparatus is suitable for experiments with silicates, metals, and solidified gases. These new methods will facilitate the study of mineral physics under experimental conditions that duplicate the natural conditions of the earth's interior.

Editor's Note: Brief summaries of significant new experimental or theoretical results of interest to the mineral physics community are welcome. Please send information to the Mineral Physics News Editor.

### Meetings

### International Mineralogical Association Meeting

The 14th General Meeting of the International Mineralogical Association (IMA) will be held in Stanford, Calif., July 13–18, 1986. Several symposia at this meeting will be of special interest to the mineral physics community. These sessions include

- Mineralogical Applications of Synchrotron Radiation
- Structural Classification of Minerals
- Thermodynamics and Kinetics of Mineral Reactions
- Ordering, Transformations, and Modulated Structures in Phyllosilicates
- Structural and Magnetic Phase Transitions of Minerals
- Physics and Chemistry of Mantle Minerals
- Applications of solid-state Nuclear Magnetic Resonance (NMR) to Minerals
  - Defect Structures in Minerals
- Electron Microscopy of the Kinetics of Mineral Transformations

In addition, symposia will focus on specific mineral groups, petrology of igneous rocks, optical microscopy, industrial mineralogy, and other topics. Plenary lectures by Ekhard Salje on the application of order parameter theory to the thermodynamic properties of phase transitions and by Ian Jackson on the elasticity of mantle minerals will also be of special interest to mineral physicists.

For additional information on the IMA meeting, write IMA 1986, Department of Geology, Stanford University, Stanford, CA 94305.

# Quantum Theory and Experiment Applications

On July 21–26, 1986, a conference on quantum theory and experiments applied to solids will be held in College Park, Md. This conference will bring together theoreticians and experimentalists from the fields of mineralogy, geophysics, solid-state physics, and chemistry. Its objectives are

• to examine the capability of various theoretical methods, including solid-state band theory, ionic model simulation, molecular cluster theory, and qualitative MO band theory for explaining the properties of solids,

• to present recent experimental data on solids at extreme pressure and temperature, defect solids, glasses and surfaces to which the above methods may be applied, and

• to focus on some particular topics of current and future interest to mineralogists and other solid-state scientists.

For more information, contact the organizers: Jack Tossell (Department of Chemistry, University of Maryland, College Park, MD 20742) or G. V. Gibbs (Department of Geological Sciences, Virginia Polytechnic Institution and State University, Blacksburg, VA 24061).

# Lithosphere and Asthenosphere

An International Workshop on Anisotropy and Inhomogeneity of the Lithosphere and Asthenosphere will be held on September 8–13, 1986, at the Castle of Bechyně, Czechoslovakia. The conference is being organized by the Geophysical Institute of the

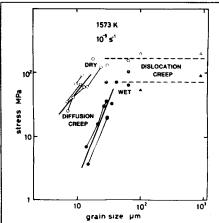


Fig. 4. Experimental determination of the boundary between the regimes in which diffusion and dislocation creep dominate the deformation of synthetic olivine aggregates. In the diffusion creep regime (small grain size, low stress), the flow stress is sensitive to grain size, and the flow is approximately Newtonian. In the dislocation creep regime (large grain size, high stress), the flow stress is insensitive to grain size, and the strain rate varies as the third or fourth power of stress. The presence of water lowers the flow stress in both regimes, as may be seen by comparing the stress-grain size curves for dry and wet specimens (Karato, Paterson and Fitz Gerald).

Czechoslovakia Academy of Sciences and the Institute of Geophysics of Charles University in Prague.

The first part of the workshop will focus on three-dimensional seismic mapping of the lithosphere and asthenosphere and on the generation of propagation of seismic waves within anisotropic and inhomogeneous media. The rest of the meeting will be devoted to considering experimental data and their application to the interpretation and implications of the velocity variations in the mantle. Mineral physics has much to contribute to this latter discussion, and anyone interested in participating in the workshop is encouraged to contact V. Babuška, Geophysical Institute, Czechoslovakia Academy of Sciences, 141 31 Prague 4 - Spořilov, Czechoslovakia; Telex 121330 or R. C. Liebermann, Department of Earth and Space Sciences, State University of New York, Stony Brook, NY 11794.

### High-Pressure Research Applications Seminar

The United States-Japan seminar on "High-Pressure Research Applications in Geophysics and Geochemistry" was held in Honolulu, Hawaii, January 13-16, 1986, under the auspices of the National Science Foundation (NSF) and the Japan Society for the Promotion of Science (ISPS). The seminar, the third in a series, was cocovened by Murli H. Manghnani (University of Hawaii, Honolulu) and Syun-iti Akimoto (University of Tokyo). Coming together for this symposium were 25 researchers from Japan, 22 from the United States, and four others, from Australia, the People's Republic of China, the Netherlands, and the Federal Republic of Germany. Of the 52 papers presented, 38 were presented orally at seven scientific sessions, and the rest were displayed at a poster session.

The scientific sessions covered a variety of state-of-art experimental techniques and theoretical topics:

• High-Pressure Techniques and Melting Experiments

• Shock Wave Experiments

Synthesis, Phase Equilibria, and Thermodynamic Properties of Mantle Phases
 Spectroscopy at High Pressure

Application of Synchrotron Radiation

Lattice Dynamic Studies

 High-Pressure Research Applications in Geophysics and Geochemistry (poster session)

 Geophysical and Geochemical Constraints In the opening lecture, Akimoto reviewed the past, present, and future of high-pressure research in geophysics, emphasizing the progress made over the past 25 yr in his laboratory at the University of Tokyo's Institute of Solid State Physics. The highlights of the recently developed high-pressure techniques were the melting and phasing transition studies that used laser- and resistance-heated diamond anvil cells (DAC). In the former case, good progress has been made in determining temperature gradients and distribution (D. L. Heinz and R. F. Jeanloz, University of California, Berkeley; W. A. Bassett et al., Cornell University, Ithaca, N.Y.); in the latter case, the P-T ranges have been improved significantly by using sintered diamond anvils (S. Endo et al., Osaka University, Osaka, Japan), by fabricating the DAC body with superalloys (D. Schiferl et al., Los Alamos National Laboratory, Los Alamos, N.Mex.), and by effecting the internal heating in a vacuum (Schiferl et al; L. C. Ming et al., University of Hawaii). The high temperature-pressure calibration, based on the pressure and temperature dependance of the lifetime of the R<sub>1</sub> fluorescence line of ruby (Y. Y. Sato-Sorensen, University of Washington, Seattle), and the optical strain measurements in DAC (Jeanloz and C. Mead, also at University of California, Berkeley) should prove to be useful in future DAC studies.

The large-volume apparatus facilities for high-pressure-high-temperature research are located principally in Japan. Further improvements in the design of such apparatuses are currently being made, and new techniques are being developed to generate higher pressures and temperatures, to 30 GPa and 2500°C (O. Fukunaga et al., National Institute for Research in Inorganic Materials (NIRIM), Ibaraki, Japan; E. Takahashi, Okayama University, Misasa, Japan). A large-volume apparatus with a truncated split sphere is also currently in use at the Australian National University (E. Ohtani et al., Ehime University, Matsuyama, Japan), thanks to the cooperation between Japan and Australia. The recent acquisition of a similar apparatus, as well as a DIA-6 apparatus, at the State University of New York (SUNY), Stonybrook (R. C. Liebermann et al.), should also open up new opportunities in the United States.

Recent applications of synchrotron radiation (SR) to high P-T research employing both DAC and large-volume multianvil (MAX80) apparatus, notably in Japan, have resulted in refinement of the equations-ofstate for garnets (T. Yagi et al., Tohoku University, Sendai, Japan) and allowed kinetics studies of the olivine-spinel phase transition in Mg<sub>2</sub>GeO<sub>4</sub> and the B1-B2 transition in KCl (G. Will and J. Lauterjung, University of Bonn, Bonn, Federal Republic of Germany). New results on the equation-of-state study of Fe and the ε transition (Akimoto et al.; Manghnani et al.; Bassett et al.) show that the phase diagram of Fe is not yet established. The SR applications also provide new opportunities for investigating the physical properties, such as viscosity, of melts at high pressure (T. Fujii et al., University of Tokyo) and for high-pressure structural studies using extended X ray absorption fine structure (EX-AFS) and X ray absorption near-edge spectroscopy (XANES) (O. Shimomura et al.,

Problems related to Fe and the earth's core were also addressed in a number of experimental studies that used both diamond anvil cell and large-volume apparatuses (H. K. Mao and P. M. Bell, Geophysical Laboratory of the Carnegie Institute of Washington, D.C.; Ohtani; S. Urakawa et al., Nagoya University, Nagoya, Japan), as well as shock wave techniques (J. D. Bass et al., University of Illinois, Champaign-Urbana; T. J. Ahrens et al., California Institute of Technology (Caltech), Pasadena, Calif.). One shock wave study, on peridot (J. M. Brown et al., University of Washington), dealt with the velocity distribution and phase transitions in the mantle. Y. Syono et al. (Tohoku University, Sendai, Japan) reported a direction-dependent shock-induced transition in single-crystal TiO2 that occurred between 13.7 and 33.8 GPa.

Among the silicate phases of the deep man-

tle, MgSiO<sub>3</sub> perovskite received the most attention. The single-crystal growth of perovskite (E. Ito and D. J. Weidner, Oakayama University) and its thermodynamic properties (E. Knittle, University of California, Berkeley, and Jeanloz), as well as the thermochemical and spectroscopic properties (A. Navrotsky, Princeton University, Princeton, N.J.) and structural transformations and thermoelastic properties (G. H. Wolf and M. S. T. Bukowinski, University of California, Berkeley), were presented in light of the nature of the deep mantle. The thermochemical and spectroscopic studies of pyroxenoids and the high-pressure polymorphs of germanate garnets, ilmenites, and MgSiO<sub>3</sub> perovskite (Navrotsky) shed new light on the garnet-to-ilmenite transition in germanates and the ilmeniteto-perovskite transition in MgSiO3. The vibrational modeling supports the idea that perovskite-forming transitions have negative P-T slopes (Navrotsky). Other high-pressure spectroscopic reports included one on the use of Raman study for phase transformations in ZrO<sub>2</sub> at high temperatures (H. Arashi, Tohoku University) and another on Raman and reflection spectra study of the pyrite system (N. Mori and H. Takahashi, University of Tokyo). Also, R. J. Hemley (Geophysical Laboratory, Carnegie Institution) presented data on the pressure dependence of phonon spectra of SiO<sub>2</sub> phases (quartz, coesite, stishovite, and silica glass) from an experiment using high-pressure Raman spectroscopy. The results were elegantly supported by quasi rigid ion lattice dynamical calculations. Y. Matsui (Okayama University) dealt with the experimental computer synthesis of silica with the -PbO<sub>2</sub> structure, and R. G. Burns (Massachusetts Institute of Technology, Cambridge, Mass.) reported on the site incompressibilities of transition metal oxides as deduced from crystal field data.

Another study of the thermodynamic properties of the mantle phases was concerned with the phase boundaries among  $\alpha$ ,  $\beta$ , and  $\gamma$ Mg<sub>2</sub>SiO<sub>4</sub> (T. Ashida et al., Osaka University, Osaka, Japan). H. Watanabe (State University of New York, Stony Brook) discussed the physiochemical properties of olivine and spinel solid solutions in the system Mg<sub>2</sub>SiO<sub>4</sub>-Fe<sub>2</sub>SiO<sub>4</sub>. Geophysical implications for mantle models, especially for the region at 400-670 km, were discussed in light of the pyroxenegarnet transformation, investigated over the range 4.6-18 GPa at 1200°C in a large-volume apparatus (A. E. Ringwood and T. Irifune, Australian National University) and by calorimetric methods (M. Akaogi et al., Kanazawa University, Kanazawa, Japan).

In reporting the new equilibrium data on  $MgSiO_3$  to 25 GPa and 2300°C, H. Sawamoto (Nagoya University) showed that pyrolite is unrepresentative of the mantle as a whole. He also reported that the 550-km discontinuity is caused by the pyroxene to garnetlike transformation and that the slope of garnet-perovskite is positive.

By using a split sphere type of ultrahighpressure apparatus, E. Ito and E. Takahashi (Okayama University) obtained new data on the phase equilibria in the systems MgO-FeO-SiO<sub>2</sub> and CaSiO<sub>3</sub>-MgSiO<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub> and in natural peridotite to 27 Gpa at 1600°C. One of their principal findings was the dissociation of the spinel solid solution (Mg1-x, Fex)<sub>2</sub>SiO<sub>4</sub> (x < 0.3) with the negative clapeyron slope. It was strongly suggested that this dissociation is responsible for the 670-km discontinuity. Mao and Bell reported new compressibility data on grossularite and andradite, with bearing on the transition zone. M. Kumazawa et al. (University of Tokyo), on the other hand, discussed the tectonic, thermal, and geochemical state inferred from the stable phases around the 670-km ir the mantle. By using this information together with the melting data, they concluded that the 670-km discontinuity is a chemical boundary.

In an overview, Don Anderson (Caltech) discussed a number of petrological models of the mantle that satisfy geophysical constraints and addressed other critical issues in mantle chemistry and dynamics. On the basis of elasticity data, Weidner argued for a uniform mantle composition.

A number of issues concerning the upper mantle and the crust were also addressed. On the basis of a melting study of peridotite to 20 GPa (E. Takahashi et al.), it was proposed that the upper mantle peridotite was generated originally as a magma (or magmas) by partial melting of the primitive earth at depths of 400–500 km. Interesting ideas concerning the generation of magmas, arc volcanism, and convection were presented by Y. Ida (University of Tokyo). S. Karato (also at University of Tokyo) proposed a number of mechanisms that cause velocity anisotropy in the mantle. It now appears that the dynamic and tectonic (stress field) mechanisms play an important role in velocity anisotropy.

The ultrasonic and static P-V measurements of selected transition metal oxides (e.g., Fe<sub>2</sub>O<sub>3</sub>) provided a good comparison of the equations of state derived by the two methods (Liebermann and A. R. Remsberg, State University of New York, Stony Brook). Similarly, the single-crystal X-ray measurements on MgF<sub>2</sub> and FeF<sub>2</sub> to 4.5 GPa were found to be in agreement with the ultrasonic equation of state (N. Nakagiri et al., University of Hawaii).

In summary, it was an opportune time for the scientists from the United States, Japan, and other countries to exchange ideas and to discuss the new advances, techniques, and results in high-pressure research in geophysics and geochemistry. The enhancements of the capabilities and improvements in the high PT ranges of both the DAC and large-volume apparatus now make possible experimentation under mantle-core conditions (with DAC) and under the conditions of the lower part of the upper mantle and the transition zone (with large-volume apparatus). It is worth noting that the thrust of petrological/ geochemical research in large-volume apparatus in Japan has certainly paid off. Yet, although our understanding of the earth's deep interior has improved and the modeling techniques for it have become more refined, all the geophysical constraints cannot as yet be satisfied because of the lack of some crucial high-PT laboratory data for certain important mineral phases that are present. Thus exciting opportunities in high-pressure mineral physics lie ahead.

This report was contributed by Murli H. Manghnani, University of Hawaii, Honolulu; Syun-iti Akimoto, University of Tokyo; Thomas J. Ahrens, California Institute of Technology, Pasadena, Calif.; Yasuhiko Syono, Tohoku University, Sendai, Japan, Raymond Jeanloz, University of California, Berkeley; and Takehiko Yagi, University of Tokyo.

### Chairman's Corner

### **Mineral Growth**

Mineral physics, like its sister disciplines geochemistry, petrology, and crystallography, is a derivative of the old discipline of mineralogy. At the turn of the century, mineralogy was one of the strongest pillars in the European University, but it was weakened by the loss of these branches, which declared their independence as they matured. One of the most important roots of solid state physics also branched off from 19th-century mineralogy.

Yet solid state physics, bound securely in the Physics Department, developed in a way that took it further and further from the interests of geological sciences. In the late 1960's, it became evident that a gap existed in laboratory and theoretical geophysics that was not filled by the then-existing disciplines of solid state physics or mineralogy. To fill this gap, it was required that the principles of solid state physics be applied to minerals of especial interest to geophysics.

The gap was wide but not vacant. Francis Birch of Harvard published several classic papers in the early 1950's and 1960's that demonstrated the power of using solid state principles to attack problems of the solid earth interior. Birch became the role model for a later generation who called themselves mineral physicists.

The path pioneered by Birch was settled by scientists who by and large stayed within the geophysical community and published especially in the AGU journals. Logically, they could have published in physics journals or in mineralogy journals. That they chose to publish mostly in geophysics journals may have been because they were united with other geophysicists in coordinated attempts to understand properties and processes of the earth's interior.

Even within the American Geophysical Union, those following Birch's path found themselves to be slightly out of step with others in the traditional disciplines of geophysics. The focus on physical properties of rockforming minerals did not harmonize easily with a focus on geophysical phenomena (e.g., earthquakes, volcanos, etc.). The extrapolation from atomic properties to global properties was made along a different trajectory than the one used by seismologists, geodesists, and volcanologists.

For a long while, the followers of the Birch tradition had no disciplinary name, and they were identified in national and international programs under such appellations as "physical properties of earth's interior" or "physical properties of geologic materials." It became important, therefore, to find a name that could capture the spirit and flavor of scientists who worked on physical problems of rock-forming minerals. At the occasion of their organization within AGU, the designation "mineral physics" was adopted, although with some reluctance because it did not include some reference to chemistry. Among the members of the Mineral Physics Committee, the word "chemistry" is always implied,

just as work in geochemistry is always implied in the title "American Geophysical Union."

In Birch's classic paper "Elasticity and Constitution of the Earth's Interior" (Journal of Geophysical Research, vol. 57, pp. 227–286, 1952), he presented several avenues of analysis:

• the calculation of P ( ) by means of an equation of state;

• the determination of thermal properties from seismic properties by the use of classical

solid state equations;

• the determination of nonhomogeneous regions from seismic data and the identification of some of those inhomogeneities as high-pressure phase changes arising in olivine and pyroxene, "possibly close-packed oxides of magnesium, silicon, and iron, similar in structure to corundum, or rutile, or spinel"; and

• the analysis of seismic data coupled with solid state equations to support the hypothesis of a predominantly iron core.

Shortly after publishing this historic paper, Birch published other important papers: one showed the significance of shock wave measurements to bear on the question of core constitution, and in another, he introduced the idea that physical properties of rockforming minerals are controlled primarily by density. In his 1952 paper, he anticipated the direction of present theory on equations of state by his statement that "as yet, there are no complete quantum-mechanical studies for materials likely to be important in the interior of the earth," clearly implying the need for this work.

These research directions formulated or anticipated by Birch still guide much of the work of mineral physicists. This is seen by the contents of the recent report [by William A. Bassett of Cornell University, Ithaca, N.Y.], called "Mineral Physics: Atomic to Global," a summary of which will be published soon in Eos. The Mineral Physics Committee of the American Geophysical Union issued their Lake Arrowhead study, which described future research opportunities for the late 1980's and 1990's. In this report a number of fundamental questions about the nature and dynamics of the earth's interior were described, and the contribution that mineral physics can make to the solution of these questions were listed as work in the following areas:

• The equation of state;

• Elastic and anelastic properties;

• High-pressure/high-temperature crystallography;

• Phase transformation;

• The nature and movement of melts;

• Theoretical modeling;

• Transport properties and crystal defects;

• Inelastic deformation;

- Mineral magnetism;
- Behavior of hydrogen and helium at high pressure and temperature;
- The state of iron in the interiors of terrestrial planets;
- Partitioning of lithophilic elements in the lower mantle;

• Core-mantle boundary

Since about half of these topics were introduced by Birch, a claim can be made that mineral physics as a discipline has a continuous record of 30 years, although a formal recognition is only 3 years old.

Orson L. Anderson Chairman, AGU Mineral Physics Committee

# WHAT'S NEWS FROM AGU

### Mineral and Rock Deformation: Laboratory Studies The Paterson Volume

336 Pages \$40 List Price

### Geophysical Monograph 36

B. E. Hobbs and H. C. Heard, Editors

ISBN: 0-87590-062-3

Introducing the latest addition to the American Geophysical Union's respected Geophysical Monograph Series, this volume focuses on various aspects of the deformation of rocks and minerals. These are the sixteen outstanding papers in this book:

Dilatancy of Quartz Gouge in Pure Shear B. Raleigh and C. Marone

The Laboratory Study of Seismic Wave Attenuation 1. Jackson

The Plasticity of Some Fine-Grained Aggregates of Olivine at High Pressure and Temperature *P. N. Chopra* 

Deformation Behavior of Wet and Dry Clinopyroxenite in the Brittle to Ductile Transition Region J. N. Boland and T. E. Tullis

Experimental Control of the Water-Weakening Effect in Quartz A. Ord and B. E. Hobbs

High Temperature Creep of Single Crystal Galena (PbS) S. F. Cox

Effect of Cation Impurities on Steady-State Flow of Salt H. C. Heard and F. J. Ryerson

Experimental Deformation of Rocksalt J. Handin, J. E. Russell, and N. L. Carter

Dynamic Recrystallization of Minerals J. L. Urai, W. D. Means, and G. S. Lister

Phase Transformation Under Stress and Volume Transfer Creep H. W. Green II

Deformation Induced Recrystallization of Ice: The Application of in Situ Experiments C. J. L. Wilson

Some Speculations on the Nature of High-Angle Grain Boundaries in Quartz Rocks A. C. McLaren

Variable Sensitivity Piezometric Equations for Dislocation Density and Subgrain Diameter and Their Relevance to Olivine and Quartz R. J. Twiss

Complete Fabric Analysis of Some Commonly Observed Quartz C-Axis Patterns S. M. Schmid and M. Časey

Heterogeneous Strain in Axial Deformation of Limestone, Textural Evidence H.-R. Wenk, H. Kern, P. Van Houtte, and F. Wagner

Experimental Rock Deformation Techniques T. E. Tullis and J. Tullis

**TO ORDER,** write or call AGU. AGU staff are available from Monday through Friday, 9 a.m. to 5 p.m. EST to take orders. Orders under \$50 must be prepaid by check, money order, or credit card. AGU accepts American Express, VISA and MasterCard. Remember, AGU members receive a 30% discount off list price.

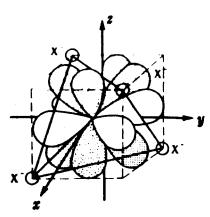
Write: American Geophysical Union

2000 Florida Avenue, NW Washington, DC 20009

Call: 800-424-2488 toll free 202-462-6903 in DC or outside the contiguous US

# **READ ALL ABOUT IT!**

# Mineral Physics News



Mineral Physics News: The focal point for the numeral physics community.

**Editor:** Robert M. Hazen, Carnegie Institution of Washington, Geophysical Laboratory, 2801 Upton Street, N.W., Washington, DC 20008 (telephone: 202-966-0354).

### Mineral and Rock Physics at the Institut de Physique du Globe de Paris

Jean-Paul Poirier

The Institut de Physique du Globe de Paris (IPG) was founded in 1921. Geophysics at that time consisted mostly of geomagnetism and the still-young seismology. The physical properties of earth materials appeared only as material constants in equations, and the fact that they were mostly unknown was not a cause for inordinate worry. Geochemistry joined the IPG program in the 1960s. When Claude Allegre became director of the institute in 1976, he saw the need for the study of the properties of minerals and rocks in their own right, as well as for the application of the recent advances in materials science to earth sciences. He then asked Jean-Paul Poirier to start a group for physics of geomaterials at IPG. Nine years later, the laboratory has become a recognized component of IPG, with interests and collaborations both in geophysics and geochemistry. The group consists of Poirier's own team (about a dozen people, including the graduate students), along with the growing teams of newcomers Yan Bottinga and Pascal Richet.

The graduate students, a numerically important fraction of the group, come from the various graduate programs in which members of the group teach: geophysics, geochemistry and materials Science. Mutual teaching among students of different backgrounds is indispensable and is done cheerfully. Some research in rock physics, including experiments in the field, is also done in the geomagnetism and seismology groups.

### Physics of Mantle Minerals

Mineral physics of the earth's mantle is one of the major research topics in the group. The instrumentation acquired or developed over the years now includes a laser-heated diamond anvil cell. X ray diffraction apparatus. and a 200-keV transmission electron microscopy (TEM)/scanning TEM electron microscope with analytical attachment (which is shared with the Laboratory of Mineralogy and Crystallography of the University of Paris 6). Techniques for the examination of the high-pressure phases produced in the diamond anvil cell (DAC) by transmission electron microscopy (TEM) were developed, mostly thanks to the skill and ingenuity of Jean Pevronneau (in charge of the DAC) and Michel Madon (TEM), with a view toward obtaining direct microstructural information on the high-pressure phases.

Michel Madon and François Guyot use these techniques to investigate the high-pressure phase transition mechanisms of olivine (olivine-spinel and postspinel transitions) and the lattice defects (dislocations, stacking faults) present in the phases. An important finding is that the transformation of olivine or spinel into perovskite and magnesiowustite takes place by a eutectoid reaction, producing alternate lamellae of MgSiO<sub>3</sub> and of MgO with a high dislocation density (Figure 1). There seems to be no reason why the mechanism observed in the DAC could not be operative at the 670-km discontinuity. Parallel investigations are under way on germanate analogues Mn<sub>2</sub>GeO<sub>4</sub> and Ca<sub>2</sub>GeO<sub>4</sub>, on the possible role of intermediate phases with K2NiF4 structure, and on the partitioning of iron between phases using the analytical attachment on the TEM.

This program involves various fruitful collaborations with A. Revcolevschi (Orsay University) for the preparation of germanates and crystal chemisty expertise, H. Boyer (lobin Yvon Company, Paris) for micro-Raman spectroscopy, and A. Putnis (Cambridge University, Cambridge, U.K.) for high-resolution TEM (under a North Atlantic Treaty Organization (NATO) grant). A cooperative research program with R. C. Liebermann's group (State University of New York at Stony Brook) on the mechanism and kinetics of olivine-spinel transition has been started. The experiments will be done in the new largevolume, high-pressure facility at Stony Brook and the products will be examined by TEM at IPG. This program is jointly funded by the Centre Nationale de la Recherche Scientifique (CNRS, France) and the U.S. National Science Foundation (NSF). In addition, Pascal Richet, who has returned from the Geophysical Laboratory, Carnegie Institution of Washington, is beginning to get equipment for determining high-pressure equations of state of minerals by using the DAC and a conventional X ray generator.

Poirier has recently applied dislocation melting theory to the determination of the melting entropy, volume, and temperature of iron. By using elastic moduli of the inner core obtained by seismology, a temperature of 5000 K is calculated for inner core bound-

ary on the basis of Lindemann's law, in good agreement with extrapolation from shock wave experiments.

## Rheology of High-Pressure Ices

The dynamics of the large icy satellites of the gas giant planets (e.g., Ganymede, Titan) depend on the viscosity of the high-pressure phases of ice. To determine this important parameter experimentally, Christophe Sotin developed a sapphire anvil cell, similar to the DAC but with a larger volume, in which pressures up to more than 20 kbars can be achieved (Figure 2). Deformation markers flow outward along the pressure gradient, and from their recorded motion the creep rate of ices can be determined.

Sotin used a nonlinear global inversion method to obtain all the parameters of the creep law (e.g., activation energy and volume, as well as stress dependence). The viscosity of ice VI has been determined to be lower than  $3 \times 10^{14}$  poise, a value that is consistent with evacuation of heat by convection in Ganymede. Investigation of the creep of ice V and ice III is underway.

### Creep of the Lower Mantle

MgSiO<sub>3</sub> perovskite is thought to be the major mineral of the earth's lower mantle, yet nothing is known of its creep properties. Indeed, almost nothing is known of the high-temperature mechanical properties of crystals

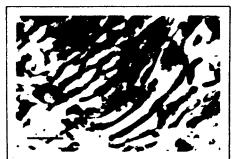


Fig. 1. Alternate lamellae of magnesiowustite (black) and perovskite formed in the DAC by eutectoid decomposition from olivine. Transmission electron micrograph. Scale bar:  $0.1~\mu m$ .



Fig. 2. High-pressure in the sapphire anvil cell. The pressure decreases from the center toward the edge. At the center is ice V, then ice III, and water near the edge (diameter of the hole: 1.5 mm).

with perovskite structure. Solange Beauchesne investigates the high-temperature creep properties of single crystals of BaTiO<sub>3</sub> and KTaO<sub>3</sub> with apparatus from the Laboratorie de Physique des Matériaux (CNRS, Bellevue, France). The results are inverted to yield a creep law based on a global inversion method developed for creep by Sotin.

Preliminary results on BaTiO<sub>3</sub> are consistent with non-Newtonian power law creep (contrary to previous experiments on fluoride perovskite KZnF<sub>3</sub>) on crystal planes (100) or (110) slip systems. TEM examination of deformed samples (Figure 3) shows dislocations with <110> and <100> Burgers vectors.

On a more macroscopic scale, Poirier and Liebermann recently showed that the variation with depth of the activation volume for creep could be calculated from seismologically obtained elastic moduli of the lower mantle and that an isoviscous lower mantle had to be somewhat superadiabatic.

### TEM Micropetrography

Most of our information on natural rocks is at the scale of optical microscopy; mineral components smaller than ~10 microns cannot generally be identified and examined. TEM can provide this data down to almost 10 A, and with electron diffraction and in situ microanalysis, it is a valuable source of information. Jannick Ingrin investigated pyroclastic ejecta from the 16th-century eruption of the Grande Soufrière volcano, Guadeloupe (French West Indies). From study and analysis of glassy inclusions in plagioclase, he obtained microscopic evidence for magma mixing, with the injection of hot basic magma in the chamber possibly triggering the eruption. Pyroclastic glass from the 1979 eruption of La Soufrière volcano on the island of St. Vincent (British West Indies) showed phase separation at the scale of 100 Å. Francois-Regis Martin-Lauzer reproduced this texture in an unmixed synthetic glass and used TEM and microanalysis to obtain an experimental mis-

Jean-Philippe Renaud has begun a TEM and analytical study of the refractory inclusions in the Allende meteorite. Investigation of the microstructure of minerals at a submicron scale may reveal significant features (such as inclusions of other minerals or exsolutions) and, through examination of the dislocation configurations, provide clues to the formation of these primitive objects.

### Liquid Silicates

The physical properties of silicate melts are a topic extensively investigated by Bottinga and Richet. Analyses of data in the literature have led to models for calculating density as well as for deriving the compressibilities of simple melts. An experimental program of heat capacity determinations from drop calorimetry measurements has been initiated by Richet and is being continued with a three-fold purpose:

• to establish a data base that is sufficiently comprehensive to allow reliable predictions of the heat capacities of silicate glasses and liquids as a function of temperature and comrosition:

• to derive the thermodynamic properties, such as absolute entropies or Gibbs free energy, of liquid silicates by thermochemical methods; and

• to study quantitatively the liquid-glass transition, the understanding of which is central to the interpretation of the differences between the properties of glasses and liquids.



Fig. 3. (110) dislocations in a single crystal of KTa0<sub>3</sub> deformed in creep at 1350°C (0.99 T<sub>t</sub>). Scale bar: 0.1 μm.

In addition to constraining thermodynamic modeling of silicate melts more effectively, these results allowed successful testing of the Adam and Gibbs configurational entropy theory of relaxation processes, as applied to the viscosity of molten silicates. An interesting feature of this theory is that the configurational entropy affects the viscosity so strongly that it could be directly determined from viscosity data (Figure 4). Checking this possibility, however, requires more data for some properties than is currently available. In particular, low-temperature heat capacity data for glasses are too scarce, and measurements are being made in cooperation with R. Robie and B. Hemingway at the U.S. Geological Survey (Reston, Va.). In addition, an apparatus will be shortly set up to measure systematically the viscosity of supercooled liquids in the range 500-900°C, i.e., at very low fluidi-

The physical and chemical properties of liquid silicates are strongly dependent on composition, and experimentation at high temperature and pressure requires a considerable investment. Bottinga has therefore started a program of theoretical investigations that aims to predict property composition systematics and to calculate quantities that are experimentally difficult or impossible to measure. The theoretical approach encompasses both classical and statistical thermodynamics. The most important recent result obtained with classical thermodynamics is the demonstration of the anomalous variation with pressure of the compressibility of silicate liquids with well-developed random network structure. The statistical thermodynamics approach is used to study liquids by molecular dynamics and Monte Carlo methods.

# Rock Physics in the Laboratory

A small group in the Laboratory of Geomaterials has recently begun investigating the physical properties of porous sedimentary rocks by using ultrasonics techniques. Vo Thanh Dung continues the program that he started with Amos Nur at Stanford University (Stanford, Calif.). He studies the attenuation of sound (in the kilohertz range) in porous rock samples saturated with various fluids by using the resonant bar technique. He specifically investigates the effect of the fluid viscosity on attenuation, and he has demonstrated the importance of the viscous shear relaxation at the interfaces. Maris Zamora seeks to obtain systematic information on the variation of the  $V_p/V_s$  ratio (or equivalently, Poisson's ratio) with the geometry of porosity, saturation, and uniaxial stress. She simultaneously measures  $V_p$  and  $V_s$  (in the megahertz range) in two perpendicular directions on the same core. Poisson's ratio ap-

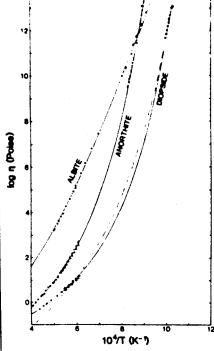
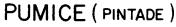


Fig. 4. Viscosity of molten albite, anorthite, and diopside as a function of temperature. Experimental data and theoretical curves (solid lines) calculated with the equation  $G = A + B T_{conf}$ . This equation gives a good fit to the experimental data over 12 orders of magnitude of viscosity and accounts for the strongly composition dependent, non-Arrhenian character of the viscosity.



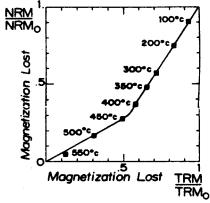


Fig. 5. Natural remanent magnetization as a function of thermal remanent magnetization at various temperatures for a pumice sample (Pintade) from the Soufrière de Guadeloupe volcano. The temperature of the deposits (450°C) can be determined from the position of the knee in the curve.

pears to be a very sensitive clue to the extent and orientation of microcracking.

Jacques Zlotnicki, of the Laboratory of Geomagnetism, is currently investigating the physics of magnetization in rocks. He uses an amagnetic triaxial press with confining pressure up to 1.5 kbar to study piezomagnetism. He finds that the magnetization of the rock is a good marker of the paleostresses and that the maximum deviatoric stress undergone by a rock sample can be determined with an accuracy of 10%–20%. Another interesting method uses measurement of thermal remanent magnetization at various temperatures;

Ziotnicki is thus able to determine the temperature of emplacement of volcanic depinal (Pyroclastic flows) when no carbonized woul can be found (Figure 5).

. . . . . . .

### Rock Physics in the Field

Concurrently with his laboratory experiments, Zlotnicki works with the IPG Volcanological Observatories to monitor the volcano-magnetic events on the Soufriere de Guadeloupe, Montagne Pelee (Martinique) and Piton de la Fournaise (Reunion) volcanos. He also uses Grand Maison Dam, in the Alps, as a field laboratory for the study of piezomagnetic signals during filling and empiying of the reservoir. Francois Cornet of the Laboratory of Seismology does in situ experimentation on forced fluid flow through a granitic massif at an experimental site in Massif Central, France; hydraulic injection tests provide reliable data for in situ stress determination.

Paris was built with limestone dug from underground quarries, and one of these disused quarries currently happens to be right under a landfill site. Pierre Morat of the Laboratory of Geomagnetism, together with the Paris Public Works Department, uses this quarry as an experimental site. The pillars are instrumented for electrical and strain measurements, and Morat measures the electrical potential variations during loading of the roof of the quarry. The measurements will be performed until the roof collapses; the results will lead to better understanding of seismoelectric signals.

Jean-Paul Poirier is with the Physics of Geomaterials Group at the Institut de Physique du Globe, Paris.

### **Opinion**

### Chairman's Corner: Current Thrust in Mineral Physics

Several positive factors have generated significant momentum and research activities in mineral physics: the interdisciplinary nature of the field, newly aroused interest through scientific communications at meetings and symposia, advancements in high-pressure/high-temperature instrumentation, and above all, commitments by individual scientists and institutions.

In the last 6 months, a number of themes in mineral physics were highlighted at the International Mineralogical Association meeting at Stanford University (Stanford, Calif., July 13–18, 1986), at the conference on "Quantum Theory and Experiment Applied to Solids" at University of Maryland (College Park, Md.; organized by J. A. Tossell and G. V. Gibbs), and at the 1986 AGU Fall Meeting (San Francisco, Calif., December 8–12, 1986). The following report discusses the highlights of the recent AGU meeting only.

Seven oral and poster sessions focused on the following themes in mineral physics:

- Rock Properties
- Synthetic Rocks
- Advances in High-Pressure Research
- Spectroscopy and Mineral Chemistry
- Silicate Liquids and Glasses
  Defects and Deformation
- Material Properties of Mantle and Core

The poster session on rock properties provided a view of diversified research on tuffs, rick salt, amphibolite, sandstone, granite, gabbros, and other rick types. The parameters and properties reported were microstructure, permeability, stress strain relations, electrical conductivity, internal friction, water weakening, and crack healing.

A timely session on synthetic rocks dealt with various theoretical and experimental aspects of hot pressing aggregates of minerals and rocks. In particular, the elastic and rheological properties of such aggregates were considered. One objective of this session was to investigate the possibilities of using synthetic aggregates for studying rock properties in the same manner that synthetic single crystals are used to study minerals. The roles of deviatoric stresses and of preferred orientation of these properties, as well as the influence of phase transformation kinetics were addressed.

Advances in experimental high-pressure research were marked by measurements and observations to 100 GPa (1 Mbar) and higher in diamond anvil cells (DAC). Energy-dispersive X ray diffraction measurements on crystalline xenon that used synchrotron radiation revealed a new solid-solid phase transition. Luminiscence and synchrotron X ray-induced fluorescence in ruby were also described. Progress in high P-T research with DAC also included equation of state and phase studies on NaCl (B1-B2) and Sn (B-II) and pressure calibration using ruby lifetime measurements. These techniques should enable a new class of high P-T experiments to become feasible in the near future.

New theoretical contributions were reported on a number of fronts, notably on the applications of the Birch-Murnaghan equation at high temperature and the calculation of  $K_0$  and  $K_0$ ' from vibrational frequencies and, for a number of oxides and silicates, lattice dynamical calculations. For oxides (especially, MgO and CaO) calculations by three different ab initio theories (linearized augmented plane wave (LAPW) band calculations and both rigid ion and breathing ion electron gas theories of crystals) were presented. A detailed comparison among the three approaches indicates very good agreement.

The poster session on spectroscopy and mineral chemistry included infrared, nuclear magnetic resonance (NMR), and Mössbauer studies of Mg-Fe silicates and mixed layer illite/smectite. Investigations of structural, substitutional, and oxidation-dehydroxylation of olivines, pyroxenes, amphiboles, mellilites, and phyllosilicates were described. Also presented were results on the spectral reflectance of mafic silicates and phyllosilicates and the effects of their dehydration, as well as the characterization of biogenetic carbonate minerals by Raman spectroscopy.

Exciting papers were presented in the poster session on silicate liquids and glasses. In addition to new instrumentation developed for high-temperature spectroscopy, studies on glasses and liquids at high temperatures, and improved pistons for the piston cylinder apparatus, experimental results on the physical properties of melts were reported. These studies included shock wave compression of molten Ano. 36 Dio. 64, compositional dependence of the densities of K2O-Na2O-Ca0-MgO-Al<sub>2</sub>O<sub>5</sub>-TiO<sub>2</sub>-SiO<sub>2</sub> liquids, ultrasonic velocities and compressibilities of Na2O-Al2O3-SiO<sub>2</sub> melts, and the effect of CO<sub>2</sub> on the viscosity and solidus of liquid silicates at high pressure.

Also reported were new high-temperature NMR results for crystalline, glassy, and molten alkali silicates and albite, Raman spectro-

scopic data for olivine composition and hydrous quartz-albite glasses, and infrared data for the D<sub>2</sub>O containing rhyolite glass. Theoretical studies included molecular dynamic models and studies of thermodynamic properties of SiO<sub>2</sub> phases and glasses.

A CANADA CONTRACTOR DE CONTRACTOR DE LA CANADA DEL CANADA DE LA CANADA DEL CANADA DE LA CANADA DEL CANADA DE LA CANADA DEL CANAD

The papers presented in the session on defects and deformation dealt with a variety of topics in rock physics bearing on crustal deformation and mantle flow properties: creep and plastic deformation in albite and anorthite rocks, pressure dependence of creep in olivine, chemically assisted cracking in quartz, and vield strength of MgO. Two other reports were on the oxidation of favalite at high temperatures and on the solubility and diffusivity of carbon in San Carlos olivines, with implications for upper mantle evolution. Finally, advances toward high-precision internal friction  $Q^{-1}$  measurements on San Carlos olivine and new low-frequency  $Q^{-1}$  results for calcite rocks as functions of pressure, frequency, and grain size were reported.

In terms of new experimental data from samples under extreme pressure and temperature conditions, the session on material properties of the mantle and core generated much excitement. The synthesis of perovskite at static pressures above 100 GPa in a laserheated diamond anvil cell was described, and K<sub>0</sub> and K<sub>0</sub>' were reported. One conclusion of this work is that silicate perovskites make up nearly 50% of the earth. Intracrystalline partitioning of Fe in synthesized perovskites, determined by extended X ray absorption fine structure (EXAFS) spectroscopy, led to the surprising conclusion that Fe substitutes for Si. This result implies that some of the Si in Mg-Fe perovskites is in higher than octahedral coordination. Melting curves of Fe and FeSb to over 100 and 60 GPa, respectively, on the basis of static experiments in a laserheated DAC, were also presented. Static results on Fe are in excellent agreement with shock wave measurements. From these static and dynamic results the first experimental constraints on core temperatures have been made. Static compression measurements on y-Ni<sub>2</sub>SiO<sub>4</sub> in a DAC, ultrasonic determinations of K<sub>0</sub> of FeO, and of the pressure and temperature derivatives of Ci of MnO, and Brillouin scattering elastic data for phlogopite were also reported.

The phase transition studies in Fe10%Ni that used synchrotron radiation and in MnTiO<sub>3</sub> from the ilmenite to the LiNbO<sub>3</sub> structure with large-volume cubic anvil apparatus were presented.

New shock wave studies have advanced our knowledge of material properties, including the melting curve of stishovite, the equation of state of serpentine to 120 GPa, and the equation of state of molten anorthite and diopside. In addition to the exciting implications for densification of melts, the latter work also promises to elucidate the coordination number changes in melts undergoing dynamic compression.

A theoretical paper focused on the manybody forces and elasticity of oxides and olivines. Models of mantle mineralogy based on bulk elastic properties are limited because we lack elasticity data for many mantle minerals. In a nutshell, mineral physics is flourishing in both experiment and theory. There is al-

ready an overlap of pressure-temperature regimes spanned by the static and dynamic experiments on one hand and by theory and experiment on the other. Further progress and a better understanding of the nature, composition, and thermal state of the earth are in store for us.



Murli Manghnani Chairman, Mineral Physics Committee

# News & Announcements

# Olivine-Spinel Transition and the 400-km Discontinuity

The sequence of high-pressure phase transitions  $\alpha$ -olivine  $\rightarrow \beta$ -modified spinel  $\rightarrow \gamma$ spinel is commonly used as a model for upper mantle seismic velocity increases in the 200-650-km depth interval. The widths of seismic transition zones and the corresponding divariant (e.g.,  $\alpha + \beta$  and  $\beta + \gamma$ ) mineral stability fields are important criteria for correlating velocity variations with phase changes. Divariant mineral stability fields are poorly known for mantle molar Mg/(Mg + Fe) ratios (about 0.9), but C. R. Bina and B. J. Wood of the Department of Geological Sciences, Northwestern University (Evanston, Ill.), have demonstrated that these fields can be constrained by requiring the Mg2SiO4-Fe2SiO4 phase diagram to be consistent with known thermochemical data. They have derived an internally consistent phase diagram (Figure 1) based on available calorimetric, thermoelastic, and synthetic data. They find that the divariant transition a  $\rightarrow \alpha + \beta \rightarrow \beta$ , which is generally regarded as occurring over a broad depth interval, is in fact extremely sharp. For mantle olivine compositions the transition takes place over a pressure interval of only about 2 kbar. The sharpness of this transition, claim the authors, is quite insensitive to uncertainties in the constraining thermodynamic data.

Bina and Wood conclude that the seismic discontinuity corresponding to the  $\alpha \to \beta$ transition in (Mg<sub>0.9</sub>Fe<sub>0.1</sub>)<sub>2</sub>SiO<sub>4</sub> should occur over a depth interval of 3-9 km at a depth of approximately 400 km. Recent seismic work indicates that the 400-km seismic discontinuity must be quite sharp, of the order of 6 km wide. Comparison of available seismic profiles derived from high-resolution waveform modeling to profiles computed from the new phase diagram and the elastic properties of the olivine polymorphs indicates that a substantial amount of olivine is required to produce a sharp 400-km discontinuity in the mantle. An upper mantle composed of about 70% olivine is required for consistency with the available velocity constraints.

# The Mineral Physics Committee

Mineral Physics Committee members for the period July 1, 1986, to June 30, 1988, have been announced. They are Murli H. Manghnam (Hawan Institute of Geophysics, Honolulu), and Orson L. Anderson (University of California, Los Angeles), Thomas J. Ahrens (California Institute of Technology, Pasadena, Calif.), Subir K. Banerjee (University of Minnesota, Minneapolis), William A. Bassett (Cornell University, Ithaca, N.Y.), Gordon E. Brown, Jr. (Stanford University, Stanford, Calif.), Michael Brown (University of Washington, Scattle), Robert M. Hazen (Geophysical Laboratory, Washington, D.C.), Raymond F. Jeanloz (University of California, Berkeley), Robert C. Liebermann (State University of New York (SUNY), Stony Brook). Alexandra Navrotsky (Princeton University, Princeton, N.J.). Robert N. Schock (Lawrence Eivermore National Laboratory, Livermore, Calif.), and Donald J. Weidner (SUNY Stony Brook).

Note: The editor of Mineral Physics News welcomes contributions of news items of interest to the mineral physics community.

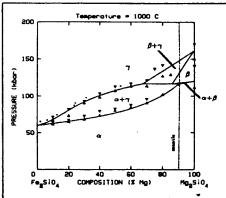


Fig. 1. Isothermal pressure-composition diagram showing calculated boundaries for olivine polymorph stability fields at 1273 K. Also shown are experimental data points delimiting the high-pressure stability limits of the low-pressure assemblages (upward pointing triangles), the low-pressure stability limits of the high-pressure assemblages (downward pointing triangles), and the compositions of  $\gamma$  phase that coexist with  $\alpha$  phase at the indicated pressures (dots). Dashed vertical line indicates the composition Mg/(Mg + Fe) = 0.9.

### Rock and Mineral Physics Register 1986/1987

This register is the first compilation of current research activity in the field of rock and mineral physics within Great Britain and Ireland, it contains details of over 50 active research groups/laboratories and nearly 150 individual scientists. It aims to provide a link by which interested researchers can readily review the current expertise and facilities available. Fields of interest include physical and themical properties, structure, phase relations, reaction mechanisms, deformation and defects, electron microscopy, modeling studies, and spectroscopic techniques.

The register was compiled by Philip Meredith and Paul Dennis of the Department of Geological Sciences at University College London and is published by the Mineralogical Society of Great Britain and Ireland. Copies have been provided free to all members of the society, but additional copies are available to both members and nonmembers from the office of the Society at 41 Queens Gate. London SW7 514R. U.K. The price, \$5.00 (U.S.), includes the mailing fee.

### Meetings

# Mineral Physics in Europe

At the next meeting of the European Union of Geophysics (EUG) in Strasbourg, France, on April 13–16, 1987, a symposium on mineral physics topics is being convened by J. P. Poirier (Institut de Physique du Globe, 4 Place Jussieu, 75230 Paris Cedex). Those interested in attending the meeting are encouraged to write directly to Poirier or to contact the foreign secretary of the Committee on Mineral Physics (R. C. Liebermann, Department of Earth and Space Sciences, SUNY, Stony Brook, NY 11794) for further details.

# Physical Properties and Thermodynamic Behavior of Minerals

A North Atlantic Treaty Organization (NATO) Advanced Studies Institute on this topic will be held in Pembroke College, Cambridge University, Cambridge, U.K., July 27–August 8, 1987. The purpose of the meeting is to promote collaboration between mineralogists, solid state physicists and chemists, and mineral scientists, and to spread awareness of methods available for studying the physical properties of minerals.

Inquiries should be addressed to the director of the institute: E. Salje, Department of Earth Sciences, Downing Street, Cambridge CB2 3EQ, U.K.

Mineral Physics (cont. from p. 179)

### Physical Properties of Solid and Molten Earth Materials

The International Association for Seismology and Physics of the Earth's Interior (IASPEI) will hold a symposium on physical

properties of solid and molten earth materials at the 1987 meeting of the International Union for Geodesy and Geophysics (IUGG), to be held in Vancouver. Canada, August 17–19, 1987. The symposium is intended to encompass all major areas of topical research into the physical properties of rocks, minerals and their melts, and their geophysical applications, including

• studies of solid-solid and solid-liquid phase equilibria and transformation mechanisms, along with structure and bonding in high-pressure crystalline and melt phases;

 bulk elastic and thermophysical properties, including equations of state, elastic moduli, vibrational spectra, thermal expansion, and Gruneisen's parameter;

• transport properties, including diffusion, anelasticity, rheology and rock deformation, electrical conductivity, and melt viscosity.

For more information, please contact the convenor, Thomas J. Ahrens, Seismological

Laboratory 252-21, California Institute of Technology, Pasadena, CA 91125.

### International Conference on Electronic Structure and Phase Stability in Advanced Ceramics

Argonne National Laboratory will sponsor a conference to be held at the laboratory (Argonne, Ill.) during August 17–19, 1987. The development of a basic science perspective for the advanced ceramics that are needed in modern high-technology systems is a major challenge to physicists, chemists, ceramists, and materials scientists. The conference will explore relationships in the following areas:

• Electronic structures of ceramic materials, including both quantum theoretic and experimental studies,

 phase equilibria calculated from firstprinciples methods with critical comparison to experimental results,

 phase stability and phase transformation examined by theoretical and experimental probing of the statics and dynamics of crystal lattices.

The conference program will include both invited and contributed lectures in these subject areas. For further information about programs and abstract submission, contact S.-K. Chan, Chairman of Organizing Committee, Materials Science Division, Building 212, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439.

# AGU Chapman Conference on Perovskites: A Structure of Great Interest to Geophysics and Materials Science

A Chapman Conference on the structure and properties of perovskites will be held in Bisbee, Ariz., on October 30-November 3, 1987. The conference will bring together experts from the fields of geophysics and materials science to discuss the complexities of this structure type in terms of its energetics. structure, bonding, phase equilibria, electrical and magnetic properties, elasticity, defects and dislocations, and reactions. An interdisciplinary approach to the physics and chemistry of perovskites will develop new insights and methods for understanding and predicting the properties of the earth's lower mantle, which probably consists largely of an MgSiO<sub>3</sub> perovskite phase.

For more information, please contact the convenor, Alexandra Navrotsky, Department of Geological and Geophysical Sciences, Princeton University, Guyot Hall, Princeton, NJ 08544. To be placed on the mailing list to receive the call for papers and other meeting circulars, write to MMP: Perovskites Chapman, 2000 Florida Avenue, N.W., Washington, DC 20009. Note that the call for papers was also presented in the November 11,

1986, issue of Eos.

### Call for Mineral Physics News and Announcements

Mineral Physics News appears biannually in Eos. News, notes, reviews, or other material of general interest to AGU and to the mineral physics community are welcome. Please send information to the editor of Mineral Physics News.

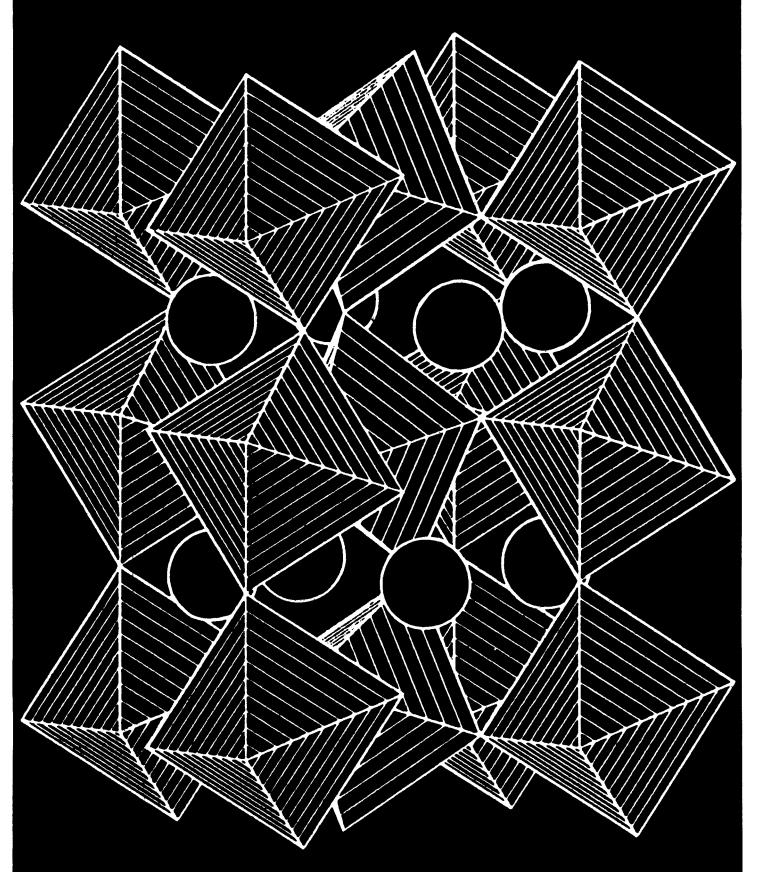
GRL Call for Mineral Physics Papers

The editors of Geophysical Research Letters (GRL) are attempting to increase submission rates in the fields of solid earth geophysics and, in particular, in mineral physics. GRL, which is noted for its record of rapid publication, welcomes short, original articles of new results presented in a way that will make their significance apparent to the general geophysics community.

For information call 202-462-6903

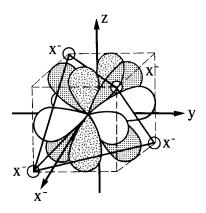


Transactions, American Geophysical Union Vol. 69 No. 2 January 12, 1988



The Commonest Mineral?

# Mineral Physics News



Mineral Physics News:

The focal point for the mineral physics community.

**Editor:** Robert M. Hazen, Carnegie Institute of Washington, Geophysical Laboratory, 2801 Upton Street, N.W., Washington, DC 20008 (telephone: 202-966-0334).

# MAX80: Large-Volume High-Pressure Apparatus Combined With Synchrotron Radiation

Takehiko Yagi

Around the world there are many highpressure devices coupled to synchrotron radiation sources. Of these facilities, MAX80 (for multianvil high-pressure X ray system) at the Photon Factory (the synchrotron radiation laboratory at the National Laboratory for High-Energy Physics in Tsukuba, Japan) has a unique capability for experiments that are simultaneously high pressure and high temperature. Because of MAX80's large sample chamber, a resistance heater can be installed so that the specimen can be heated uniformly to 1600°C at pressure. Scientists have employed this apparatus for in situ X ray observations of phase transitions, measurements of silicate melts, and other high-pressure experiments.

### The Apparatus

As described briefly in a previous Mineral Physics News [Liebermann et al., 1985], MAX80 consists of a DIA-10 cubic anvil high-pressure vessel, a 500-ton hydraulic ram, goniometer, solid-state detector, and data acquisition system (Figure 1). Additional details of the system are given by Shimomura et al. [1985, 1987] and Yagi et al. [1987]. White synchrotron X radiation enters the sample chamber through gaps in the tungsten carbide an-

vils, and diffracted X rays pass through the opposite gap where they can be measured by the solid-state detector. This apparatus is designed to obtain powder diffraction profiles via the energy dispersive technique. Furthermore, the small divergence of the incident beam allows the use of X ray shadowgraphs, which are especially useful in studying the properties of silicate melts.

A typical sample assembly is shown in Figure 2. The pressure-transmitting medium and heater are made of a boron epoxy resin mixture and graphite, respectively. Temperature is measured by a thermocouple, while pressure is calculated from the lattice parameter of an internal standard material, such as NaCl or Au. The pressure-temperature range attainable by MAX80 depends on the size of the anvils. Truncations of the anvils are from 12 to 3 mm on edge, yielding maximum pressures from 3 to 12 GPa, respectively. Smaller anvils yield higher pressures. The maximum attainable temperature at 12 GPa has been 800°C, while 1600°C has been sustained at 6 GPa. Efforts to extend the pressure range by adopting sintered diamond anvils are in progress. To date, pressures as high as 60 GPa at room temperature have been achieved [Endo et al., 1987], and high-temperature experiments within this pressure range are now being attempted.

The storage ring at the Photon Factory is usually operated at 2.5 GeV, and high-energy X rays up to 35 KeV are available at the bending magnet beam line. When the vertical wiggler line is used, this energy range is extended to more than 80 KeV and the intensity is increased by a factor of 10. This high intensity and wide energy range make it possible to observe many high-quality diffraction lines from each sample. Recently, MAX80 has

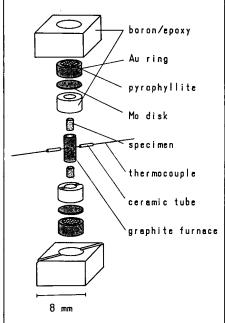


Fig. 2. Standard sample assembly for high-pressure and -temperature experiment.

been placed on an accumulator ring that is operated at 6 GeV, which further extends X ray energies to 130 KeV, with the same high X ray flux that is possible on the wiggler line.

### The Experiments

MAX80 is uniquely suited for a number of experiments of interest to the geophysical

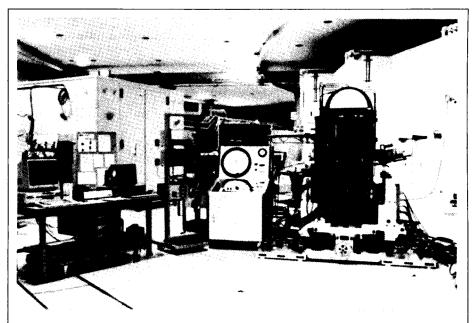


Fig. 1. MAX80 high-pressure and high-temperature X ray diffraction system. From right to left: high-pressure unit, pressure controller, temperature controller and multichannel pulse height analyzer, and data acquisition system. The high-pressure unit is installed in a sealed room during the experiment.

community. As stated above, the large sample chamber allows installation of an internal heater that provides simultaneously high-temperature, high-pressure environments for a relatively large sample (several cubic millimeters). Such a large sample provides adequate material for X ray diffraction from relatively light-atom silicates. Furthermore, silicate melting at high temperature and pressure can be documented, and melt viscosity can be measured by X radiography of falling metal spheres. Many physics, material sciences, and earth sciences studies have been carried out with MAX80. Some examples relevant to mineral physics are summarized below.

### In Situ Observations of Phase Transformations

Phase transformations in silicates play an important role in the formation of a layered structure and in consequent seismic discontinuities of Earth. An understanding of these phase transitions are thus important in characterizing the solid Earth. Phase transformations in silicates have been studied by using quench experiments, but the information obtained through these experiments has been limited by uncertainties associated with cooling. By using the MAX80 system, it is possible to perform detailed in situ observations of transformations. Information on transition pressures, density changes at the transition, and equations of state of different phases can be obtained with an accuracy not heretofore available. Accumulation of phase transition data provide a more complete picture of the structure of Earth's deep interior.

One example of this kind of research is the study of the olivine-spinel transformation in Fe<sub>2</sub>SiO<sub>4</sub> by Yagi et al. [1987a]. Diffraction profiles obtained in this study are shown in Figure 3. It is clear from these figures that highquality X ray diffraction patterns for these materials can be obtained in short exposure times, typically 200 seconds, and the progress of phase transitions can be clearly observed. In this example a mixture of olivine and spinel phases was kept at 5.1 GPa and 800°C. By repeating the observation every 200 seconds, relative stability of the two phases was compared. Unit cell volumes of each phase can also be calculated from these diffraction patterns. The data were used to calculate an accurate phase boundary, kinetics of the transformation, and equations of state of the two

One interesting phenomenon found in this research is that thermal expansion of a quenched high-pressure phase observed at room pressure differs significantly from that observed at high pressure under the stable conditions. This effect may occur because a partial retrogressive transition took place under metastable conditions, and the crystal expanded slightly. To avoid complexities of this type, the unit cell volume of the specimen should be measured carefully both before and after the temperature cycle as a check for permanent changes in the lattice parameter.

### **Equations of State of High-Pressure Minerals**

The most important observations from Earth's deep interior are seismic velocities. Elastic properties of high-pressure minerals

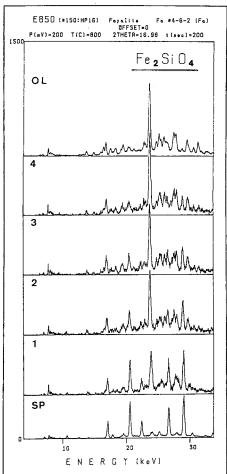


Fig. 3. Diffraction profiles of Fe<sub>2</sub>SiO<sub>4</sub>. OL and SP represent the single phases of olivine and spinel, respectively. When the mixture of these two phases (panel 1, at the bottom) was kept at 5.1 GPa and 800°C, it transformed into a single phase of olivine, over time (panels 2–4). Exposure time of each diffraction profile is 200°C.

are therefore among the most important properties to measure in the laboratory. Unfortunately, most high-pressure minerals are synthesized in a small sample chamber, and it has proven difficult to obtain reliable equations of state by using conventional powder diffraction methods. For example, many recent Earth models predict the existence of large amounts of majorite (garnet structure with a composition corresponding to a pyroxene-garnet solid solution), but little was known about the elastic properties of majorite

The use of synchrotron radiation has made it possible to determine reliable equations of state from several-milligram powder specimens. As an example, isothermal compression curves of pyrope and enstatite-pyrope solid solution measured by MAX80 [Yagi et al., 1987b] are presented in Figure 4. From these observations it became clear that by dissolving the pyroxene component into the garnet structure, the bulk modulus became smaller than that of the garnet end-member, a result contrary to previous experiments. These results for high-pressure minerals provide new constraints on the constitution of Earth's deep interior.

### Structure and Physical Properties of Silicate Melts Under Pressure

Silicate melts play an essential role in many geophysical phenomena. Because of the experimental difficult, however, little is known about the structure and physical properties of these melts under pressure. MAX80 has provided a new means of studying these problems.

The high intensity, high signal-to-noise ratio, and wide energy range of this X ray system have made it possible to measure diffraction profiles of silicate melts under pressure. Figure 5 is an example of a profile obtained on jadeite at 3.6 GPa. The starting material

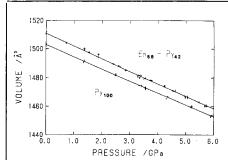


Fig. 4. Isothermal compression curves of pyrope and estatite-pyrope solid solution (majorite) at room temperature. The length of each cross represents the error bar of the measurements. By dissolving the pyroxene component into garnet, the unit cell and the compressibility of garnet increase slightly.

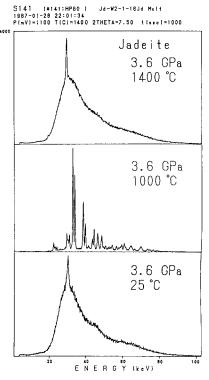


Fig. 5. Diffraction profiles of jadeite. When the glass specimen was heated at 3.6 GPa, it crystallized into jadeite at about 1000°C and then melted at about 1400°C. The sharp peak observed at 25°C and at 1400°C is the diffraction from the graphite capsule.

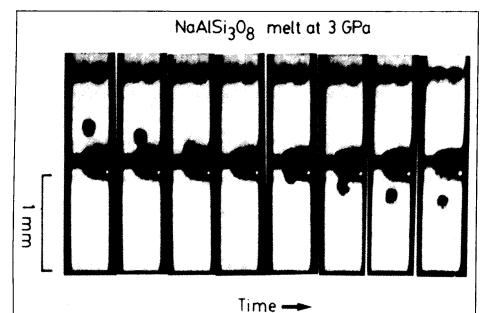


Fig. 6. X ray shadowgraphs of a platinum sphere sinking in molten albite at about 3 GPa. The time interval of each photograph is 20 s. The radius of the platinum sphere is 90 µm, and the horizontal shadow in the center is produced by the thermocouple outside of the capsule. A viscosity of 300 poise was obtained during this experiment.

was a glass that first crystallized into jadeite with increasing temperature and then melted. Diffraction profiles of this molten silicate were compared with those obtained from a calculated diffraction pattern based on molecular dynamics simulation [Kawamura et al., 1987]. It is known that the viscosity of this melt decreases with increasing pressure, and the present study suggests that this viscosity decrease is caused by the size change of the rings that form the network and the appearance of regularly coordinated aluminum.

Viscosity and density of silicate melt under pressure are the most important yet also the most difficult properties to measure. Kushiro [1976] developed a novel method to measure these properties by using a falling sphere technique combined with a quench experiment. The method was subsequently modified by Hazen and Sharpe [1983], who used X radiography to locate the platinum and boron nitride sphere positions. The high brightness and small divergence of the synchrotron radiation are ideally suited for making X ray shadowgraphs for in situ observation of rising or falling spheres in molten silicates. Figure 6 is a sequence of photographs of such an event [Kanzaki et al., 1987] in which the shadow of a falling platinum ball is recorded by a videotape recorder, giving an accurate velocity of settling. This method has improved the accuracy of the viscosity measurements and has expanded the range of measurable viscosities considerably. When two spheres of different density are used, the high-pressure density of the silicate melt can be calculated along with the viscosity.

### **Conclusions**

Synchrotron radiation, coupled with the large-volume high-pressure apparatus, has made it possible to obtain new information on the behavior of silicates at high pressure and temperature. Accumulation of these data will result in a greater understanding of the

constitution and evolution of Earth's interior. Further efforts to extend the pressure and temperature range of the MAX80 system are in progress in the continuing effort to reproduce environments of Earth's deep interior.

### References

Endo, S., N. Toyama, A. Ishibashi, T. Chino, E. Fujita, O. Shiomura, K. Sumiyama, and Y. Tomii, Determination of α-ε transition pressure in Fe-V alloy, in High-Pressure Research in Mineral Physics, Geophys. Monogr. Ser., vol. 39 or Min. Phys. Ser., vol. 2, edited by M. H. Manghnani and Y. Syono, pp. 29–33, AGU, Washington, D.C., 1987.

Hazen, R., and M. Sharpe, Radiographic determination of the positions of platinum spheres in density-viscosity studies of silicate melts, Carnegie Inst. Washington Yearbh., 82, 428, 1983.

Kanzaki, M., K. Kurita, T. Fujii, T. Kato, O. Shimomura, and S. Akimoto, A new technique to measure the viscosity and density of silicate melts at high pressure, in *High Pressure Research in Mineral Physics, Geophys. Monogr. Ser.*, vol. 39 or *Min. Phys. Ser.*, vol. 2, edited by M. H. Manghnani and Y. Syono, pp. 195–200, AGU, Washington, D.C., 1987.

Kawamura, K., T. Yagi, E. Takahashi, H. Maekawa, and Y. Matsui, High-pressure structural study of the NaAlSi<sub>2</sub>O<sub>6</sub> melt, paper presented at the Spring 1987 Materials Research Society Symposium, Anaheim, Calif., 1987.

Kushiro, I., Changes in viscosity and structure of melt of NaAlSi<sub>2</sub>O<sub>6</sub> composition at high pressure, J. Geophys. Res., 81, 6347, 1976

Liebermann, R. C., C. T. Prewitt, and D. J. Weidner, Large-volume high-pressure mineral physics in Japan, Eos Trans. AGU, 66, 138, 1985.

Shimomura, O., S. Yamaoka, T. Yagi, M. Wakatsuki, K. Tsuji, O., Fukunaga, H. Kawamura, K. Aoki, and S. Akimoto, Multianvil type x-ray apparatus for synchrotron radiation, Mater. Res. Soc. Symp. Proc., 22, 17, 1984.

Shimomura, O., et al., Multi-anvil type x-ray system for synchrotron radiation, in *Solid State Physics Under Pressure*, edited by S. Minomura, pp. 351–356, KTK/Reidel, Tokyo/London, 1985.

Yagi, T., M. Akaogi, O. Shimomura, T. Suzuki, and S. Akimoto, In situ observation of the olivine-spinel transformation in Fe<sub>2</sub>SiO<sub>4</sub> using synchrotron radiation, *J. Geophys. Res.*, 92, 6207, 1987a.

Yagi, T., M. Akaogi, O. Shimomura, H. Tamai, and S. Akimoto, High pressure and high temperature equations of state of majorite, in *High-Pressure Research in Mineral Physics, Geophys. Monogr. Ser.*, vol. 39 or *Min. Phys. Ser.*, vol. 2, edited by M. H. Manghnani and Y. Syono, pp. 141–147, AGU, Washington, D.C., 1987b.

Takehiko Yagi is at the Institute for Solid State Research, University of Tokyo.

# News & Announcements

### High-Pressure Earth Sciences Work Funded in Canada

Chris Scarfe (University of Alberta, Edmonton, Canada) has been awarded a National Scientific and Energy Research Council (NSERC) Major Installation Grant to purchase and operate high-pressure apparatus for research in geochemistry, geophysics, and materials development. The award, which was supported by Karlis Muehlenbachs and Tom Etsell (also of the University of Alberta), Mike Fleet (University of Western Ontario, London, Canada), Hugh Greenwood (University of British Columbia, Vancouver, Canada), and 15 other coinvestigators across Canada, amounts to approximately \$1 million. The University of Alberta has contributed \$250,000 plus \$60,000 for laboratory preparation and installation costs, and NSERC has provided \$521,899 in capital costs and \$210,000 in operating costs over 3 years.

The initiative represents a major step forward for experimental geochemistry and geophysics in Canada. The apparatus, developed over the last 15 years in Japan, will be the only one in Canada and the second in North America. The uniaxial split sphere apparatus (USSA) is a large hydraulic press of 2000 tons capacity. The uniaxial pressure drives multiple anvils that pressurize a sample assembly of up to approximately 1 cm<sup>3</sup> volume. Pressures can be as high as 300 kbar (30 GPa) at temperatures of up to 3000°C. These conditions allow laboratory simulation of Earth's interior down to ~800 km, a depth equivalent to the upper part of the lower mantle.

Research programs with the USSA-2000 will be directed toward understanding Earth's mantle: its composition, properties, layered structure, and evolution over the course of geological time. Comparative studies will relate the mantle of our planet to the mantles

of the other terrestrial planets. The other major research direction will be the synthesis and fabrication of "advanced materials." This is an area of rapid growth because new technologies require new materials. Some of these materials will be fabricated at high pressures, notable examples being superhard materials such as synthetic diamond and the cubic form of boron nitride. The use of diamond as a cutting tool is well known, and the applications of boron nitride in the aerospace industries are growing.

### Mineral Physics News and Announcements Wanted

The Mineral Physics News appears biannually in Eas. News, notes, reviews, or other material of general interest to AGU and the mineral physics community are welcome. Please send information to the editor of Mineral Physics News.

### Meeting Report

### AGU Chapman Conference on Perovskites

October 30 to November 2, 1987, an international group of 75 physicists, chemists, geophysicists, and materials scientists met in Bisbee, Ariz., for an AGU Chapman Conference on the interdisciplinary topic Perovskites: A Structure of Great Interest to Geophysics and Materials Science. The meeting, which followed the annual Geological Society of America convention in Phoenix, Ariz., was organized by Alexandra Navrotsky (Princeton University, Princeton, N.I.).

Perovskites, a class of compounds with the ideal formula ABX<sub>3</sub>, occur in one of the most adaptable crystal structures known to man. The ideal form, represented by the mineral perovskite (CaTiO<sub>3</sub>, which gives the group it

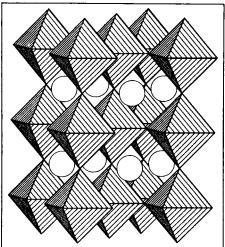


Fig. 1. The simple cubic pervoskite structure, with an ideal chemical formula ABO<sub>3</sub>, has a corner-linked array of octahedral atom clusters. Cages formed by the octahedra hold large metal atoms.

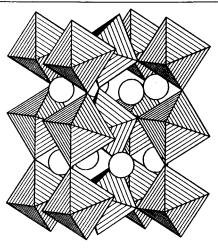


Fig. 2. Ferromagnesian silicate perovskite, (Mg, Fe)SiO<sub>3</sub>, is believed to be abundant in Earth's lower mantle. The structure is related to the simple cubic perovskite by tilting of the octahedra.

name), is among the simplest crystal structures (Figure 1). This high-symmetry structure may be altered in any number of ways, however: by slight distortion of the atomic framework, by missing atoms, by layering, and by other variations that lead to atomic arrangements of extraordinary complexity. These modifications cause many of the unique properties of perovskites. For example, perovskites are the only crystal structures that can perform as electrical insulators, semiconductors, superionic conductors, metal-like conductors, and super conductors. Thus the purpose of the meeting was to focus on the diversity and complexity of perovskites as viewed by scientists from different disciplines.

The first session featured six lectures on magnesium silicate perovskite (ideally, MgSiO<sub>3</sub>; see Figure 2), a high-pressure phase of special concern to the mineral physics community. Silicate perovskites are believed to constitute almost half the volume of the solid earth. Following a dynamic and provocative review of recent high-pressure research by Raymond Jeanloz (University of California, Berkeley), several speakers focused on aspects of silicate perovskite phase relations, rheology, structure, and compositional variation. A number of detailed experimental studies of MgSiO<sub>3</sub> perovskite have been made possible through E. Ito's (Okayama University, Okayama, Japan) synthesis of single crystals with diameters greater than 0.1 mm.

One recurrent theme of the conference arose in the first few talks: The common assumption that MgSiO<sub>3</sub> perovskite is stoichiometric at high pressure and temperature, especially in iron- and calcium-bearing varieties, has yet to be demonstrated and may well be wrong. Perovskites are commonly deficient in cations. Those defects will drastically alter key physical properties such as creep, electrical conductivity, and trace element partitioning. For many of us the success of this first stimulating session was reflected in the fact that we came away knowing a lot less about silicate perovskites than we had a few hours before.

The second session focused on perovskites as technological materials. In an invited lecture, Robert Newnham (Pennsylvania State

University, University Park) reviewed a few of the many economic applications of perovskites, which are the basis of a \$20 billion per year market. Newnham emphasized the use of three types of perovskite: barium titanate (cation-doped BaTiO<sub>3</sub>), the most widely used dielectric; PZTs (solid solutions of PbTiO3 and PbZrO<sub>3</sub>), piezoelectric ceramics; and PTC (positive temperature coefficient of resistance) materials that are used in voltage surge protectors. A paper by S. A. Sunshine (AT&T Bell Laboratories, Murray Hill, N.J.) focused on the next generation of commercial perovskites: the high-temperature oxide superconductors, all of which have structures related to perovskites (Figure 3). Throughout these and subsequent talks on perovskite thermochemistry (by Navrotsky) and reaction chemistry (by A. J. Jacobson, Exxon Research and Development), the critical effect of defects, composition, and nonstoichiometry on physical properties was stressed.

A poster session on Friday evening featured a diverse sampling of perovskite research. Papers on high-pressure silicates were juxtaposed with contributions on fluorides, germanates, and cuprate superconductors. It was especially evident at this session that high-pressure silicate perovskites must be viewed in the context of other exotic ABX<sub>3</sub>

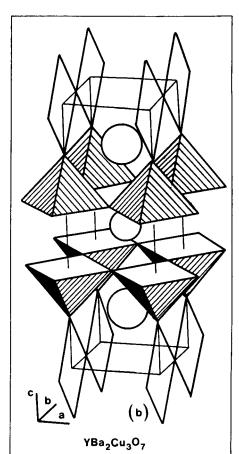


Fig. 3. The high-temperature superconducting perovskite YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> has a tripled c crystallographic axis as a consequence of barium (large circles) and yttrium (small circles), which are ordered in the sequence Ba-Y-Ba, Ba-Y-Ba, Two of every nine perovskite oxygens are absent, giving the superconductor a uniquely ordered arrangement of oxygen atoms.

compounds, rather than as just another insu-

lating silicate mineral.

The Saturday morning session was devoted to theoretical approaches to understanding perovskites. Ekhard Salje (Cambridge University, Cambridge, U.K.) discussed mechanisms and kinetics of perovskite phase transitions, noting that four different mechanisms — octahedral tilting, B cation "off-centering," covalent deformation, and A cation "off-centering" — contribute to soft mode transitions. Complex perovskite transformations may involve the interaction of two or more of these mechanisms. It was pointed out that the symmetry of metastable magnesium silicate perovskite at room conditions need not be the same as that of the phase deep within the Earth.

Salje's review was followed by four speakers who presented contrasting computer simulations of the structure and properties of MgSiO<sub>3</sub>. Subrata Ghose (University of Washington, Seattle) described rigid ion calculations to model lattice dynamical behavior. Russell Hemley (Carnegie Institution of Washington, Geophysical Laboratory, Washington, D.C.) described measurements of the pressure dependence of vibrational modes of MgSiO3 and interpreted the results with calculations based on the non-rigid ion, potential-induced breathing model. Ronald Cohen (Naval Research Laboratory, Washington, D.C.) and Hemley were able to reproduce the observed structure, equation of state properties, and vibration frequencies remarkably well with this model. Cohen also presented results of rigorous but computationally timeconsuming linearized augmented plane wave calculations of the electron structure. Finally, G. D. Price (University College London) proposed possible diffusion mechanisms in silicate perovskite on the basis of molecular dynamics simulations. It was evident from these theoretical presentations that computer simulations can aid in the interpretation of existing experimental data, was well as provide useful insights in the absence of experi-

Defects and nonstoichiometry, recurrent themes of the conference, were the focus of three Saturday afternoon papers. R. S. Roth (National Bureau of Standards, Gaithersburg, Md.) and D. M. Smyth (Lehigh University, Bethlehem, Pa.) reviewed some of the bewildering variety of perovskite-related defect structures, while Barry Wechsler (Hughes Research Laboratories, Malibu, Calif.) presented a thermodynamic model for point defects in barium titanate.

The elasticity of perovskite was featured in talks by Amir Yeganeh-Haeri and Donald Weidner (both of State University of New York, Stony Brook) and by M. Fischer (Université Pierre et Marie Curie, Paris). Yeganeh-Haeri's contribution on Brillouin spectroscopy of MgSiO<sub>3</sub> perovskite single crystals has been eagerly awaited. He presented the first experimental value of shear modulus (184 Mbar); however, the bulk modulus (245 Mbar) and axial compression ratios determined by Brillouin scattering differ somewhat from two independent single-crystal X ray measurements (which also differ from each other). These discrepancies point out the need for more synthetic crystal specimens, careful sample characterization, and independent confirmation of crucial mineral

Sunday morning's session included a potpourri of experimental reports on diverse pervoskites: Nb-Bi oxides, KMnF<sub>3</sub>, and various naturally occurring species. The emphasis on mineral perovskites provided an excellent lead-in to afternoon excursions to the historic mines and mineral localities of Bisbee, a copper mining center that was at one time Arizona's most populous town.

The final session emphasized perovskite plasticity and its relationship to microstructure. Nothing is known of the deformation behavior of MgSiO<sub>3</sub> at mantle conditions. What is certain is the the plasticity of perovskite, and by extension the convection behavior of Earth's lower mantle, is dependent on the nature and density of defects. Jean-Paul Poirier (Institut de Physique du Globe, Paris) reviewed experimental deformation studies of perovskites (mostly titanates) and extrapolated those results to silicate perovskites. Five subsequent speakers discussed recent perovskite research, including kinetic studies, microhardness tests, and transmission electron microscopy, that shed light on the complex nonequilibrium behavior of these phases.

The Chapman Conference on perovskites sent a strong message to all those in attendance. Materials research must be tackled on a broad, interdisciplinary front. Earth materials are not fundamentally different from other compounds, nor can Earth scientists afford to ignore the research of other materials scientists. In the case of ferromagnesian silicate perovskite — probably Earth's most abundant mineral — we must embrace results from both experiment and theory on a wide range of silicate and analog systems if we are to understand the structure and properties of the solid Earth.

This report was contributed by Robert M. Hazen, Carnegie Institution of Washington, Geophysical Laboratory, Washington, D.C. Hazen is also editor of the Mineral Physics News.

### Meeting Announcements

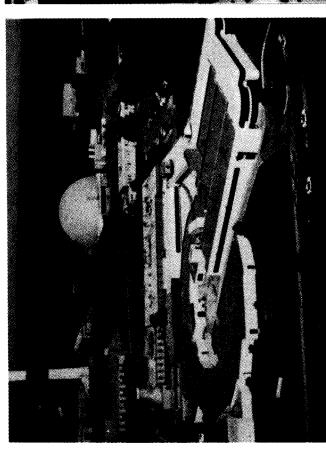
### V. M. Goldschimdt Conference

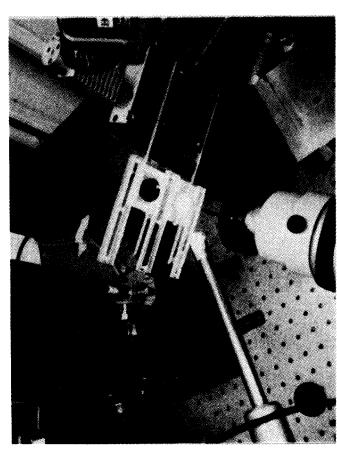
The V. M. Goldschmidt Conference, which marks the centennial year of the famous geochemist's birth, will be held May 11–13, 1988, at the Hunt Valley Inn near Baltimore, Md. The meeting is conveniently scheduled just prior to the May 15–20, 1988 AGU Spring Meeting in Baltimore.

The conference, which is jointly sponsored by the European Association of Geochemistry, the Geochemical Society, the International Association of Geochemistry and Cosmochemistry and the Mineralogical Society of America, will feature 10 symposia, two of which are of special interest to the mineral physics community. G. V. Gibbs (Virginia Polytechnic and State University, Blacksburg) is organizing a symposium entitled Modern Concepts in Crystal Chemistry, and D. H. Eggler (Pennsylvania State University, University Park) is organizing a session called Mantle Petrology and Mineralogy.

Further information is available from Goldschmidt Conference Coordinator, 410 Keller Building, Pennsylvania State University, University Park, PA 16802.

Transactions, American Geophysical Union Vol. 69 No. 52 December 27, 1988

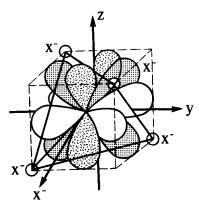




Synchrotron X-ray Sources in the Earth Sciences



# Mineral Physics News



Mineral Physics News: The focal point for the mineral physics community.

Editor: Robert M. Hazen, Carnegie Institution of Washington, Geophysical Laboratory, 2801 Upton Street, N.W., Washington, DC 20008 (telephone: 202-966-0334).

# Synchrotron X Ray Sources in the Earth Sciences

### Introduction

The importance of X rays in the Earth sciences can be traced back to 1915, when the Braggs first used this energetic form of electromagnetic radiation to determine the atomic level structures of minerals. This basic structural information is now an essential part of our knowledge about the Earth and its dynamic processes. During the past 20 years, major advances in experimental and theoretical methods, X ray instrumentation, X ray sources, and computer automation have resulted in significant gains in our ability to study the structure, bonding, and composition of Earth materials.

The recent development of synchrotron radiation sources (SRS) has provided revolutionary opportunities in the materials sciences (in its broadest sense) that are being exploited by the Earth science community. Indeed, geoscientists are leading the development of new

Cover. (Upper left): The National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory, Upton, N.Y. The NSLS has a 750-MeV storage ring which produces VUV radiation and a 2.5-GeV storage ring which produces hard X rays. (Upper right): The synchrotron X ray fluorescence trace element microprobe on beamline X-26C at the NSLS. Shown is the sample stage, optical viewing microscope with T.V. camera and Si(Li) detector. (Lower right): A scanning X ray fluorescence image of sulfide minerals (pyrrhotite, chalcopyrite, and pentlandite) from an ore deposit showing the distribution of the trace element Pd. The scan is 41 × 41 pixels with a 30-µ pixel size. The mean Pd concentration is about 100 ppm.

techniques in areas such as high-pressure physics and chemistry, X ray spectroscopy, and trace element fluorescence. SRS offer enhancements over conventional X ray sources that have led to major improvements in sensitivity and spatial resolution for a variety of analytical techniques.

The current status of research and development using SRS and future prospects were reviewed in a workshop held at Argonne National Laboratory, January 18-20, 1988, and this article is based on the report [Smith and Manghnani, 1988] by W. A. Bassett, G. E. Brown, Jr., L. W. Finger, D. L. Heinz, R. J. Hemley, A. P. Jephcoat, K. W. Jones, M. M. Manghnani, M. L. Rivers, J. V. Smith, S. R. Sutton, and G. A. Waychunas. (For a copy of this report, write to Advanced Photon Source, Argonne National Laboratory, 9700 South Cass Ave., Argonne, IL 60439.) Particularly important in the workshop report is an evaluation of the new opportunities offered by a third generation SRS—the Advanced Photon Source (APS) to be constructed at Argonne National Laboratory with commissioning scheduled for the mid-1990s.

The purpose of this article is to provide a brief overview of the current and future applications of synchrotron radiation in the Earth sciences. The GeoSync Users Committee was formed in January 1988 and affiliated with the Mineral Physics Committee of AGU in May to coordinate the use of synchrotron radiation. The cochairmen of this committee are Gordon E. Brown, Jr. (Stanford University, Stanford, Calif.) and William A. Bassett (Cornell University, Ithaca, N.Y.).

# **Synchrotron Radiation Sources**

Synchrotron radiation is the electromagnetic radiation emitted when a high-energy beam of charged particles is deflected. In a synchrotron storage ring, electrons (or positrons) are accelerated by several hundred millions of volts and injected into a closed orbit which is maintained by bending magnets. The electrons lose energy by emission of synchrotron radiation at each bending magnet, and this energy is replenished by RF cavities inside the ring. The storage ring is an ultra-high vacuum (UHV) system composed of curved sections inside bending magnets linked by straight sections. Synchrotron radiation sources differ from X ray tube sources in the much greater brightness (photons-/s/eV/µrad²), high degree of polarization, continuous spectral distribution, and time structure. Flux, brightness, and brilliance must be considered when comparing the value of various X ray sources for a particular experiment. Flux is the important parameter for an experiment with a large sample which benefits from maximizing the total number of photons. Brightness is important for small targets. High brilliance, defined as brightness per unit source area, is important when focusing optics are employed.

The first-generation storage rings were used mainly for experiments in high-energy physics, and photons were available only for short periods in "parasitic mode." Important pioneering research was done with the SPEAR ring at the Stanford Synchrotron Ra-

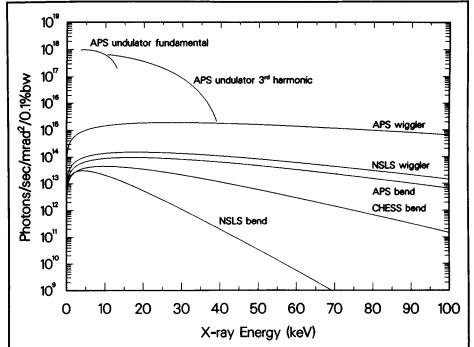


Fig. 1. Spectral distribution of some synchrotron X ray sources. Shown are NSLS bending magnet, NSLS Superconducting Wiggler, CHESS bending magnet, APS bending magnet, APS wiggler, and APS undulator. Note that the APS undulator curve is the envelope of the maximum flux from the first and third harmonics when the device is tuned over its operating range. All of the other curves are the actual spectral output under fixed operating conditions.

diation Laboratory (SSRL), and the Cornell High Energy Synchrotron Source (CHESS) at the Cornell Electron Storage Ring (CESR). The fully dedicated second-generation National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory (BNL), Upton, N.Y., has a VUV, soft X ray ring with 0.7-GeV electron energy and an X ray ring with 2.5-GeV electron energy (cover photograph). Third-generation rings are being designed specifically for high-energy wiggler and undulator insertion devices (see below). Figure 1 summarizes the spectral characteristics of some SRS.

Each bending magnet of a synchrotron storage ring emits an intense horizontal fan of polarized polychromatic radiation which is highly collimated in the vertical direction (characteristic vertical opening angles are less than 0.01°). The continuous energy spectrum is characterized by a critical energy  $E_c$  above which one-half of the total power exists. The radiation is pulsed, since it is emitted as each electron bunch traverses a bending magnet. The electron bunches are typically a few nanoseconds long and are spaced by tens or hundreds of nanoseconds. Straight sections of existing rings are being retrofitted with multiple magnets of alternating polarity, socalled insertion devices, which force electrons into a snakelike path. Wigglers produce large electron deflections (high magnetic fields) resulting in no phase coherence, but the X ray intensity is multiplied by the number of poles. Undulators produce small electron beam deflections, and phase interference occurs. This interference effectively concentrates the photon energies into narrow bands instead of the continuous spectrum emitted by a bending magnet or wiggler. Furthermore, undulator radiation is collimated in both the vertical and horizontal directions. Spectral maxima from an undulator can be tuned by varying the gap between the pole pieces thereby modifying the magnetic field. A tunable undulator is particularly valuable for experiments requiring quasi-monochromatic radiation that can be tuned through an absorption edge.

Synchrotron radiation experiments are performed on beamlines, which are vacuum systems emanating tangentially from each magnetic device in the ring. Each beamline is usually shared by a group of scientists, such as a Participating Research Team (PRT) at the NSLS. PRTs obtain the funding for construction of a beamline and operate and maintain the apparatus on a daily basis. The advantages of this approach include rapid hardware and software development, cost sharing, and fruitful scientific interactions which accompany a collaborative endeavor. A great effort is made to welcome new users who are well advised to consult with an active member of a PRT. It is wise to visit an SRS to get a "feel" for the working atmosphere before planning a detailed research project. Workshops and user meetings provide excellent introductions.

# Geological Experiments Using Synchrotron Radiation

The extremely high flux and brilliance of synchrotron X ray sources has opened up research areas in mineral physics and chemistry which are inaccessible with conventional X ray sources. Geological experiments currently

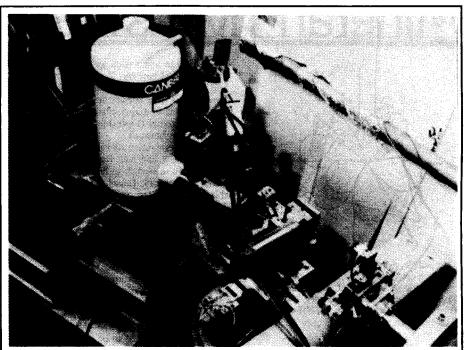


Fig. 2. Photograph of the apparatus used at beamline X-7 at the NSLS for simultaneous high-pressure, high-temperature X ray diffraction with a synchrotron source and a diamond anvil cell in the energy-dispersive mode. The sample is located between gem quality diamond anvils at the intersection of the synchrotron X ray beam and 1064 nm radiation from a Nd-YAG laser. Diffracted X rays are collected with a solid state detector, and ruby luminescence (for pressure determination) is collected by a microscope objective and dispersed onto a diode array. Both detectors must be precisely aligned with the first axis; for experiments to 500 GPa, spatial resolution down to 1 μm is required.

performed using synchrotron radiation fall into five general categories—scattering, high-pressure/temperature diffraction, spectroscopy, fluorescence, and microtomography. Examples of current research are given below for each category.

Scattering-Synchrotron sources allow X ray scattering experiments with higher-energy resolution on smaller samples than possible with conventional X ray tubes through enhanced signal-to-noise ratios. These types of measurements include powder diffraction, single-crystal diffraction, noncrystalline scattering, anomalous scattering, and surface diffraction. Higher sensitivity also permits timeresolved experiments. Structural refinements from diffraction data on individual ≈10 µm crystals are possible [e.g., Bachman et al., 1983]. The use of synchrotron radiation in powder diffraction experiments has led to dramatic improvements in resolution, peak shapes, and time required for data collection, making structure solution feasible [Prewitt et al., 1987]. The availability of synchrotron radiation has opened up high-resolution studies of interfaces in synthesized materials [e.g., Fischer-Colbrie, 1986], and the extension of this approach to geological problems is just beginning.

High P/T Diffraction—Diamond anvil cells (DAC) have achieved sustained P/T environments comparable to those found in planetary cores. Synchrotron X ray diffraction experiments (Figure 2) yield the greatest amount of information from these samples that are severely constrained by the size (less than 40  $\mu$ m) and absorption of the DAC itself. Large-volume presses can also be inserted on beamlines for more complex experi-

ments at somewhat lower pressures [Shimomura et al., 1985]. Equation-of-state measurements of H in DAC has been determined at NSLS up to 26 GPa [Mao et al., 1988], and work on other low-Z elements continues. Large-volume presses are particularly valuable for time-resolved studies of transient phenomena such as olivine-spinel transitions [Will and Lauterjung, 1987] and metal distortions [Bassett and Huang, 1987].

Spectroscopy—Absorption edge studies have greatly advanced using monochromatized synchrotron radiation for extended X ray absorption fine structure (EXAFS) and X ray absorption near-edge structure (XANES) spectroscopies. Such experiments on geological materials are impossible with conventional X ray sources because of the low concentrations. Detailed structural and bonding information has been obtained on a wide variety of geological materials including silicates, oxides, solid solutions, and metamict minerals [e.g., Brown et al., 1988]. Structures of submonolayer adsorbents on oxide surfaces in contact with water can be determined (Figure 3) [Hayes et al., 1987]. Coordination environments of cations such as Fe2+ have been studied in silicate melts and quenched glasses [Waychunas et al., 1988].

Fluorescence—The high X ray flux from synchrotron sources is ideal for X ray fluorescence determinations of chemical composition with high spatial resolution and elemental sensitivity [Hanson et al., 1987]. The brilliance of conventional X ray sources is too small to be used in an X ray microprobe. With SRS, trace element partitioning and diffusion can now be studied on the ten-\(\mu\)m scale. The microprobe at NSLS-X26 has been used to

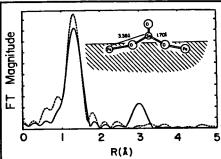


Fig. 3. Fourier transform of the Se K-EXAFS spectrum of selenite adsorbed to  $\alpha$ -FeOOH (solid line) and of selenite in aqueous solution (dashed line). The inset shows a model structure with distances which are consistent with the EXAFS data. The oxide is the striped area below the line which represents the oxide-water interface [from Hayes et al., 1987].

study platinum group element partitioning in sulfides, gold speciation in ores [Chen et al., 1987], trace element diffusion in silicate melts [Baker and Watson, 1987], siderophile partitioning in iron meteorites [Sutton et al., 1987], location of toxic elements in coal, and compositions of interplanetary dust particles [Sutton and Flynn, 1988].

Microtomography—High-resolution nondestructive mapping of the internal density distribution in solids is possible with synchrotron radiation. Work has been done by Exxon on coal [Flannery et al., 1987] and on biological specimens at NSLS-X26 [Spanne and Rivers, 1987]. Ten-µm spatial resolution has been achieved.

### Operational Synchrotron Radiation Sources

Twelve electron or positron storage rings in seven countries produce synchrotron radiation in the hard X ray range (4->50 keV), and 13 storage rings in the same countries produce synchrotron radiation in the soft X ray, vacuum ultraviolet range (1-4000 eV). Four hard X ray synchrotron sources outside of the United States have been utilized by Earth scientists in significant ways. These include LURE at Orsay, France; SRS at Daresbury, Great Britain; DESY at Hamburg, West Germany; and the Photon Factory at Tsukuba, Japan. In the U.S. there are four operational high-energy synchrotron sources that produce hard X rays: the Stanford Positron Electron Accumulation Ring (SPEAR) at the Stanford Synchrotron Radiation Laboratory (SSRL); the Positron-Electron Project (PEP) storage ring at SSRL; the Cornell High Energy Synchrotron Source (CHESS); and the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory. All of these facilities except PEP have been heavily used by Earth scientists. The total number of available hard X ray experimental stations is 58.

### SPEAR

SPEAR normally operates in a fully dedicated synchrotron mode at 3 GeV and 80 mA and occasionally in a parasitic mode at 1.8 GeV and 20 mA. Nine beamlines are supported, four with bending magnets ( $E_c \approx 4.7$  keV), four with wiggler insertion devices, and one with an undulator insertion device. A to-

tal of 22 experimental stations are available, 13 providing hard X rays and 9 providing soft X ray/VUV radiation. The soft X ray-/VUV stations provide experimental capabilities for UHV compatible studies (X ray and UV photoelectron spectroscopy, low-energy electron diffraction, surface EXAFS, X ray lithography/microscopy). The hard X ray stations provide a variety of experimental capabilities, including small- and large-angle scattering, anomalous scattering, surface scattering, single-crystal goniometers, and rotation cameras for single-crystal diffraction studies, absorption spectroscopy (EXAFS and XANES), and topography. Twenty-one stations have double-crystal monochromators or ruled gratings which enable continuous tuning of photon energies over a wide range. One white radiation station is available for high-pressure, energy dispersive X ray diffraction studies of geological materials.

#### PEP

The PEP storage ring is equipped with two synchrotron beamlines, each utilizing a 52pole undulator insertion device. This ring operates at 8 GeV in parasitic mode and up to 16 GeV in dedicated mode. Extremely low emittances and exceptionally high brilliances have been achieved in limited parasitic runs during the past year. PEP will serve as the most advanced synchrotron source during the next 8 years, while APS is under construction and will also function as a test bed for developing new types of insertion devices to be used at APS. To date, only a few Earth science projects have been proposed for PEP, and these are primarily surface-scattering or high-pressure DAC studies.

### **CHESS**

CHESS operates at 5.5 GeV and has three bending magnet beamlines (A, B, C) with critical energies of ~8.7 keV. Beamline A is also equipped with a wiggler. The three A stations offer fixed wavelength, variable wavelength, or white radiation. The B line has a single white light station. The two C line stations each can provide white or variable monochromatic radiation. X ray diffraction studies at high pressures and temperatures using diamond anvil cells have been conducted primarily with white radiation on the B line using energy dispersive techniques but also using the A wiggler. Element specific X ray radiography has been done on C.

### **NSLS**

The NSLS X ray ring operates at 2.5 GeV and 150 mA with a bending magnet critical energy of ≈5 keV. Twenty-eight beam ports are supported, each of which contains several beamlines. Thirty-seven experimental stations are operational with an ultimate capacity of 56. Several insertion devices are in use or planned. Three bending magnet ports have played important roles in Earth science research—X3, X7, and X26. X3 and X7 are being used primarily for crystallographic studies of both single-crystal and polycrystalline samples using both white and monochromatic radiation. Diamond anvil cell measurements have been made at both ports. X26 contains the X ray fluorescence microprobe using white light with monochromatic capabilities soon to be added. X17 is being constructed with a superconducting wiggler as its source.

When this line is operational, high-pressure-high-temperature research will be carried out there using diamond anvil cells, as well as a DIA-type cubic-anvil large-volume press, and high-energy X ray fluorescence microprobe measurements will be made with emphasis on rare earth elements. The X19 beamline is now being commissioned for EXAFS and XANES experiments, with an extensive program on coal properties planned.

# **Future Synchrotron Radiation Sources**

Upgrading of existing synchrotron radiation sources will continue over the next few years. These changes will include addition of beamlines and insertion devices but may also involve increases in storage ring energies and currents and reductions of emittance. For example, at SSRL, several new hard and soft X ray beamlines are currently being planned or are under construction on SPEAR. A new multipole undulator beamline is also planned for PEP. These projects should be completed by early 1990. At Cornell, construction of CHESS II began in March 1988 and will require 8-12 months for completion. CHESS II will be the mirror image of CHESS I but will support a permanent magnet wiggler capable of providing a flux 5 times greater than that produced by the CHESS I wiggler. At NSLS, 24 additional stations are scheduled to be commissioned in the near future, including the superconducting wiggler port mentioned

Over the next decade, several third-generation synchrotron sources designed specifically for insertion devices will be constructed in the U.S. and Europe. The U.S. synchrotron radiation community is planning two new facilities: the Advanced Photon Source (APS) at Argonne National Laboratory, which will operate at 7-8 GeV, and the Advanced Light Source (ALS) at Lawrence Berkeley Laboratory, Berkeley, Calif., which will operate at 1-2 GeV. The APS will accommodate 34 insertion devices and 35 bending magnets along its 1060-m circumference, positron storage ring servicing up to 100 experimental stations [Shenoy et al., 1988]. The European community is constructing the European Synchrotron Radiation Facility (ESRF) also planned for high-energy insertion devices [Burras, 1984].

Overall, 30–40 new experimental stations are planned for the next 5–7 years in the U.S. That number could easily rise to 50 or 60 as more stations are added to existing beamlines and more beamlines are added to existing sources. The commissioning of APS in the mid-1990s will make 69 additional beamlines potentially available. These next generation synchrotron radiation X ray sources will undoubtedly create new opportunities for Earth science research, and some of the obvious applications are discussed below.

### New Earth Science Opportunities With Future Synchrotron Radiation Sources

The most obvious research areas that will benefit from the next generation X ray sources are those involving low element concentrations, extremely high pressures, and temperatures and transient phenomena for which rapid data acquisition is required. Many elements of interest in Earth materials (e.g., Ar, Nd, Sm) occur at trace concentration levels (<1000 ppm), making conventional scattering or spectroscopic studies of their structural environment and bonding virtually impossible with current technology. Consequently, little is known about the distributions of these elements in mineral structures (crystallographic sites versus defect sites) or about their crystal chemical behavior (bonding, site partitioning, short-range ordering, complex formation, diffusion mechanisms, etc.). Such information is valuable in a variety of geological contexts, for example, to provide an understanding of the "blocking temperatures" of radiogenic elements and their daughter products in minerals that have undergone metamorphism. Moreover, with the gains being made in synchrotron X ray microprobe analyses of trace elements in minerals at the NSLS, there is a growing need for parallel information on crystal chemistry. X ray absorption spectroscopy (XAS) studies of such elements in bulk geologic samples are currently difficult because of insufficient flux from existing X ray sources. The new high-brilliance X ray sources that will become available in the mid-1990s will permit XAS studies of trace elements in minerals, gels, glasses, melts, and electrolyte solutions at concentration levels approaching those in natural systems and at spatial resolution levels of 1  $\mu m^2$ or less.

The study of minor and trace elements in Earth materials using the X ray fluorescence microprobe will be greatly enhanced by future SRS. The low emittance and inherent narrow energy bands of the undulators will allow the production of much smaller beams and thereby improve spatial resolution. The wigglers will produce orders of magnitude more flux at high energy than currently available, and efficient excitation of K-fluorescence from high atomic number elements will be achievable. An important result of this advancement will be the study of elemental partitioning and diffusion behavior under physical and chemical conditions which more closely simulate natural environments.

Surface studies will also be enhanced, including improved information on reactions, element partitioning, structure, and bonding at mineral surfaces and interfaces. For example, hydrolytic weakening of minerals at crack tips is of great significance in the fracturing and faulting of crustal rocks. Very little is known about these types of sites in minerals because few methods have the ability to spatially resolve and isolate such sites or to provide element specific structure and bonding information for elements in such sites at low concentrations. X ray absorption spectroscopy of cations at these types of sites should be possible with the new sources. Structural studies of chemisorption and physisorption on geologically relevant single crystals is another research area that will be accessible for the first time.

Knowledge of the structure-property relationships of minerals and fluids under extreme conditions is of critical importance in developing models of many geological processes, particularly dynamic processes in the Earth's mantle. As experimentally accessible temperatures and pressures are pushed to the values typical of those in the Earth's lower mantle and core (T>3000K, P>250 GPa),

new information on phase stability, phase transitions, and equations-of-state is gained. The large pressure and temperature gradients and small-sample volume inherent to the diamond anvil cells used in this work require very high X ray flux in a very small spot for X ray absorption and diffraction measurements.

New classes of time-resolved X ray diffraction and spectroscopy experiments (e.g., structural studies of transient phenomena such as first-order solid-solid phase transitions, melting, and higher-order transitions) will be possible. Development of the fast detection devices required for these measurements is underway [Clarke et al., 1988].

### How to Use a Synchrotron

U.S. X ray synchrotrons are user facilities and, as such, are available to new users at no charge. Several mechanisms are available to scientists who wish to conduct research at an X ray synchrotron facility. At the NSLS one can enter into a collaborative research project with an existing member of a PRT. PRTs welcome new collaborators, and this is an excellent way to become familiar with synchrotron-based research. Another mechanism available at all of the SRS facilities is to apply for beam time on a no-charge, proposal re view basis. Each beamline, whether it is owned by the SRS facility or by a PRT makes a fraction of the beam time available to general outside users. This mechanism is probably most appropriate for users who have had some previous synchrotron experience or for relatively routine types of experiments. At the NSLS a Faculty Student Support Program also exists which can provide funds to cover expenses incurred during initial experiments. For further information on the use of the X ray synchrotron facilities in the U.S., prospective users can contact the following: National Synchrotron Light Source (NSLS), Susan White-DePace, User Administrator, Building 725B, Upton, NY 11973, tel. 516-282-7114; Cornell High Energy Synchrotron Source (CHESS), Penny Ellison, 200 L Wilson Laboratory, Cornell University, Ithaca, NY 14853, tel. 607-255-7163; Stanford Synchrotron Radiation Laboratory (SSRL), Katherine Cantwell, Manager Bin 69, P.O. Box 4319, Stanford, CA 94305, tel. 415-854-3300, ext.

The following are existing or planned centers that will be operated as user facilities for members of the Earth sciences community.

### **NSLS**

Beamline X2: X Ray Tomography—Kevin D'Amico, Exxon Research and Engineering Company, Annandale, N.J.

Beamline X7: Single-Crystal Diffraction—Ake Kvick, Chemistry Department, Brookhaven National Laboratory, Upton, N.Y. Powder Diffraction—David Cox, Physics Department, Brookhaven National Laboratory.

Beamline X17: High-pressure-temperature studies with diamond anvil cells—Ho-kwang Mao, Geophysical Laboratory, Washington, D.C. High-pressure-temperature studies using a large-volume press—Donald Weidner, Department of Earth and Space Sciences, SUNY at Stony Brook, N.Y.

Beamline X19: EXAFS experiments—Barry Gordon, Department of Applied Science, Brookhaven National Laboratory.

Beamline X26: X Ray Microprobe Facility operated by the Brookhaven-University of Chicago Regional Center for Trace Element Geochemistry—Joseph V. Smith, Department of the Geophysical Sciences, University of Chicago, Ill.; Keith W. Jones, Department of Applied Science, Brookhaven National Laboratory.

### SSRL (SPEAR)

Beamline II-2: High-pressure-temperature studies using diamond anvil cells—Murli Manghnani, Hawaii Institute of Geophysics, University of Hawaii at Manoa, Honolulu.

Beamlines IV-1 and VII-2: X ray absorption spectroscopy studies over a broad temperature range—Gordon E. Brown, Jr., Department of Geology, Stanford University, Stanford, Calif.

### **CHESS**

High-pressure beamline: High-pressuretemperature studies using diamond anvil cells—William Bassett, Department of Geological Sciences, Cornell University, Ithaca, N.Y.

### References

- R. Bachman, H. Kohler, H. Schulz, H.-P. Weber, V. Kupcik, M. Wendschuh-Josties, A. Wolf, and R. Wulf, Structure analysis of a CaF<sub>2</sub> single crystal with an edge length of only 6 μm: An experiment using synchrotron radiation, Angew. Chem. Int. Ed. Engl., 22, 1011, 1983.
- D. R. Baker, and E. B. Watson, Diffusion of major and trace elements in compositionally complex Cl- and F-bearing silicate melts, in *Proceedings of the 9th University Conference* on Glass, Rensselaer Polytechnic Institute, Troy, N.Y., 1987.
- W. A. Bassett, and E. Huang, Mechanism of the body centered cubic T hexagonal close packed phase transition in iron, *Science*, 238, 780, 1987.
- G. E. Brown, Jr., G. Calas, G. A. Waychunas, and J. Petiau, X ray absorption spectroscopy and its applications in mineralogy and geochemistry, *Rev. Mineral.*, 18, 431, 1988.
  B. Burras, and S. Tazzari, Report of the Eu-
- ropean Synchotron Radiation Facility, c/o CERN, LEP Div., Geneva, Switzerland, 1984.
- J. R. Chen, E. C. T. Chao, J. A. Minkin, J. M. Back, W. C. Bagby, M. L. Rivers, S. R. Sutton, B. M. Gordon, A. L. Hanson, and K. W. Jones, Determination of the occurrence of gold in an unoxidized Carlin-type ore sample using synchrotron radiation, *Nucl. Instrum. Methods Phys. Res.*, B22, 394, 1987.
- R. Clarke, P. Sigler, and D. Mills (Cochairmen), Time-resolved studies and ultrafast detectors, Workshop Rep. ANL-APS-TM-2, 51 pp., Argonne Natl. Lab., Argonne, Ill., 1988.
- A. Fischer-Colbrie, Grazing incidence X ray studies of thin amorphous layers, Rep. 86/05, 235 pp., Stanford Synchrotron Radiation Lab., Stanford, Calif., 1986.
- B. P. Flannery, H. W. Deckman, W. G. Roberge, and D. L. D'Amico, Science, 237, 439, 1987.
- A. L. Hanson, K. W. Jones, B. M. Gordon, J. G. Pounds, W. Kwiatek, M. L. Rivers, G. Schidlovsky, and S. R. Sutton, Trace element measurements using synchrotron ra-

- diation, Nucl. Instrum. Methods Phys. Res., B24/25, 400, 1987.
- K. F. Hayes, A. L. Roe, G. E. Brown, Jr., K. O. Hodgson, J. O. Leckie, and G. A. Parks, In situ X ray absorption study of surface complexes at oxide/water interfaces: Selenium oxyanions on alpha-FeOOH, Science, 238, 783, 1987.
- H. K. Mao, A. P. Jephcoat, R. J. Hemley, L.
  W. Finger, C. S. Zha, R. M. Hazen, and D.
  E. Cox, Synchrotron X ray diffraction measurements of single-crystal hydrogen to
  26.5 GPa, Science, 239, 1131, 1988.
- C. T. Prewitt, P. Coppens, J. C. Phillips, and L. W. Finger, New opportunities in synchrotron X ray crystallography, Science, 238, 312, 1987.
- G. K. Shenoy, P. J. Vicarro, and D. M. Mills, Characteristics of the 7-GeV advanced photon source: A guide to users, *Rep. ANL-88–* 9, 52 pp., Argonne Natl. Lab., Argonne, Ill., 1988.
- O. Shimomura, S. Yamaoka, T. Yagi, M. Wakatsuki, K. Tsuji, H. Kawamura, N. Hamaya, K. Aoki, and S. Akimoto, Multi-anvil type X ray system for synchrotron radiation, in Solid State Physics Under Pressure: Recent Advances With Anvil Devices, edited by S. Minomura, pp. 351-356, D. Reidel, Hingham, Mass., 1985.
- J. V. Smith, and M. Manghnani (Cochairmen), Synchotron X ray sources and new opportunities in the Earth sciences, Workshop Rep. ANL-APS-TM-3, 127 pp., Argonne Natl. Lab., Argonne, Ill., 1988.
- P. Spanne, and M. L. Rivers, Computerized

- microtomography using synchrotron radiation from the NSLS, Nucl. Instrum. Methods Phys. Res., B24/25, 1063, 1987.
- S. R. Sutton, and G. J. Flynn, Stratospheric particles: Synchrotron X ray fluorescence determination of trace element contents, *Proc. Lunar Planet. Sci. Conf.*, 18th, 607, 1988.
- S. R. Sutton, J. Delaney, J. V. Smith, and M. Prinz, Copper and nickel partitioning in iron meteorites, Geochim. Cosmochim. Acta, 51, 2653, 1987.
- G. A. Waychunas, G. E. Brown, Jr., C. W. Ponader, and W. E. Jackson, Evidence from X ray absorption for network-forming Fe<sup>2+</sup> in molten silicates, *Nature*, 332, 251, 1988.
- G. Will, and J. Lauterjung, The kinetics of the pressure induced olivine-spinel phase transition in Mg<sub>2</sub>GeO<sub>4</sub>, in *High-Pressure Re*search in Mineral Physics, Geophys. Monogr. Ser., vol. 39, edited by M. Manghnani and Y. Syono, pp. 177–186, AGU, Washington, D.C., 1987.

This article was contributed by Stephen R. Sutton and Mark L. Rivers, Department of the Geophysical Sciences, University of Chicago, Illinois, and Department of Applied Science, Brookhaven National Laboratory, Upton, N.Y.; Joseph V. Smith, Department of the Geophysical Sciences, University of Chicago; Gordon E. Brown, Jr., Department of Geology, Stanford University, California; and Keith W. Jones, Department of Applied Science, Brookhaven National Laboratory.

This item was contributed by Catherine McCammon, Department of Geological Sciences, University of British Columbia, Vancouver, Canada.

### Synchrotron Radiation, Applications in the Earth Sciences

A report on synchrotron radiation has been prepared by the Mineral Physics Committee to inform members of the Earth science community of the potentials of this powerful new tool. The report, which was prepared by W. A. Bassett, G. B. Brown, M. H. Manghnani, H. K. Mao, and L. C. Ming will be published sometime in the next few months by AGU as a separate document. The following is a summary of its contents. Anyone wanting a copy of the report should write to Customer Service at AGU.

Synchrotron radiation has become an important and widely used tool for probing the structure, composition, and bonding of materials in all forms, including those of interest in the Earth sciences. We now have access to a broad energy continuum (1-70,000 eV) of highly collimated X rays, a billion times as bright as those produced by conventional electron impact X ray tubes. This remarkable increase in X ray brightness (number of photons per unit solid angle) has extended greatly the range of structural and chemical investigations possible, permitting studies of very dilute systems, extremely small samples, samples at extreme conditions of pressure and temperature, and phenomena of very short duration. Experiments that were considered unfeasable a few years ago (e.g., structural and compositional definition of molecular complexes on metal surfaces; real time structural studies of catalytic reactions or of solidsolid phase transitions) are now becoming routine.

At present there are four operating highenergy synchrotron sources in the U.S. that produce hard X rays: the Stanford Positron Electron Accumulation Ring (SPEAR) at the Stanford Synchrotron Radiation Laboratory (SSRL), the PEP (Positron-Electron Project) storage ring at SSRL, the Cornell High Energy Synchrotron Source (CHESS), and the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory, Upton, N.Y. The total number of experimental stations available on these sources is about 50. The number of beam lines and experimental stations at each of these facilities is planned to increase significantly over the next decade. In the mid 1990s a fifth synchrotron source, the Advanced Photon Source (APS), will become operational at Argonne National Laboratory, Argonne, Ill., adding 69 new beam lines and at least that many new experimental stations. The APS will also offer a very significant increase in X ray brightness relative to all existing sources except the PEP ring at SSRL. The increased brightness of the APS will permit new types of experiments on Earth materials that are now brightness limited (e.g., studies of samples with extremely low element concentrations). This new national synchrotron radiation facility will also offer the Earth sciences community the opportunity to take part in the planning and implementing of beam lines and experimental stations that are tailored specifically to the needs of this community.

# News & Announcements

# Mineral Physics in Canada, 1988

Mineral physics is emerging as a coherent discipline in Canada. Most laboratories have specialized in traditional mineralogy and crystallography over past years, but new laboratories are being set up that focus on research that specifically includes mineral physics. The vast size of Canada and the failure of annual meetings to attract a diverse audience of mineral physics in the past, but several initiatives in the next few years promise to change this trend.

Several universities have very strong programs in mineral physics. The Department of Geophysics at the University of Western Ontario specializes in high-pressure experiments and has a wide range of apparatus. A new split-sphere high-pressure apparatus has recently been set up at the University of Alberta in the Department of Geology. The Department of Geology at the University of Manitoba maintains a strong program in crystallography and crystal chemistry. The University of British Columbia has recently been awarded a grant to set up a shock wave facility in the Department of Physics; this complements the already existing diamond anvil lab in the Department of Geological Sciences. A more extensive list of facilities and research

in Canada is being prepared for a future submission to the Mineral Physics column in Eos.

A blow to mineral physics was struck with the tragic death of Chris Scarfe, University of Alberta, in July 1988. Chris had recently set up the second split-sphere apparatus in North America and brought the facility successfully through the testing and development phase. The future of the facility depends strongly on the person who is hired to replace his position. An international search is currently underway, and the position is planned to be filled by September 1989. Meanwhile, research is continued at the facility by graduate students and postdoctoral fellow. A Canadian SEDI (Study of the Earth's Deep Interior) Committee has been set up as part of the International SEDI group and is being chaired by David Crossley of McGill University. Mineral physics has been recognized as one area of major importance, and Catherine McCammon of the University of British Columbia has been appointed as representative. Preliminary plans include a NATO-sponsored conference at Banff to focus on Canadian research. A symposium is being organized in conjunction with the 1990 Geological Association of Canada—Mineralogical Association of Canada meeting that will be held in Vancouver. The title of the symposium is "New trends in Mineral Physics," and the focus will be on summarizing where we are with regard to outstanding problems in mineral physics. Invited speakers are from both the United States and Canada, and the major aim of the symposium will be to foster a greater collaboration among Canadian scientists in mineral physics. The proceedings will be published in a subsequent issue of the Canadian Mineralogist.

Earth science applications in which synchrotron radiation plays an important role can be divided into four general areas: X ray scattering studies of Earth materials (crystalline and noncrystalline) under ambient conditions; diffraction studies of Earth materials at high pressures and/or temperatures; spectroscopic studies of Earth materials, including X ray absorption and X ray emission spectroscopy; and spatially resolved X ray fluorescence (microprobe) studies of compositional variations in Earth materials. Another synchrotron-based method that may become important in the detection and characterization of defects and strain fields in mineral single crystals is X ray topography. Soft X ray/vacuum ultraviolet radiation (1-3000 eV) from synchrotron sources has not yet been widely used in Earth sciences research. However, great potential exists for applications of intense radiation in this energy range to problems involving the structural environments of low atomic number elements (Li to Cl) and those involving characterization of surface reactions of minerals with liquids and gases. As new methods are developed in response to increases in X ray brightness from new synchrotron radiation sources, new applications will undoubtedly result. Some of these methods will prove useful in Earth sciences research and could well be developed by Earth scientists. One can only guess what new knowledge and methods may come from synchrotron radiation research in the years ahead.

We recommend that eight new Earth sciences beam lines be planned and constructed at the Advanced Photon Source. We further recommend that the use of existing U.S. synchrotron facilities by the Earth sciences community be better coordinated so that the needs of groups of Earth science investigators with common goals can be better met. To facilitate the pursuit of these objectives and to help coordinate fund-raising efforts needed for their implementation, a new Earth sciences synchrotron users organization, Geo-Sync, has been formed.

This item was contributed by William A. Bassett, Department of Geological Sciences, Cornell University, Ithaca, N.Y.

### **Mineral Physics Award**

The Mineral Physics Committee is pleased to announce the Mineral Physics Award. This award was approved by Council at the AGU Spring Meeting. It will be used each year to encourage a promising student in mineral physics by paying his or her travel expenses to attend one of the national meetings of AGU. Although the details of the competition have not yet been established, it will probably be based on a written item submitted by the student and a letter of recommendation from the student's advisor.

Won't you please make a contribution to the Mineral Physics Award Fund. You can do this in one of two ways: send a check to AGU at any time specifying that it is for the Mineral Physics Award Fund or contribute when you pay your AGU dues. There will be a place on your dues bill to indicate the amount and destination of your contributions

If you know of some students that you think should be considered for the award,

please send their names and addresses to me, William A. Bassett, Department of Geological Sciences, Snee Hall, Cornell University, Ithaca, NY 14653. I will notify them of the rules of the competition once they have been established.

### **Meetings Featuring Mineral Physics**

The Mineralogical Society of America (MSA) will jointly sponsor several mineralphysics-related sessions at the AGU Spring Meeting, to be held in Baltimore, Md., May 8-12, 1989. In conjunction with AGU's Planetology section of AGU, MSA will host a special session on "The Mineralogy of Planetary Interiors and Surfaces." Two sessions of papers will focus on compositional and phase changes in planetary interiors, remote sensing, and in situ analyses of planetary surfaces, and chemical weathering of surface minerals. MSA and AGU's Vulcanology, Geochemistry and Petrology Section will jointly sponsor a special session on high-pressure research in memory of Chris Scarfe, a member of both MSA and AGU who was a leader in highpressure research. The AGU Spring Meeting will also feature a special session on computer modeling of crystal structures. Emphasis will be on prediction of mineral crystal structures and physical, chemical, and spectroscopic properties based on computational models of interatomic forces. In addition, MSA will sponsor a special session on mineral spectroscopy, including applications of IR, visible, Raman, X ray, and gamma ray spectroscopy to mineralogical problems, particularly those of geophysical interest. Calls for papers and other Spring Meeting news will appear in future issues of Eos.

The 28th International Geological Congress, to be held in Washington, D.C., July 9–19, 1989, will include several mineral physics sessions. Symposia on "Mineral Physics," "Ultra-High Pressure Mineralogy," "Thermodynamics and Spectroscopy," "Kinetics in Mineral Reactions," and a session on synchrotron radiation will feature more than 50 speakers. For more information, contact IGC, P.O. Box 727, Tulsa, OK 74101–0727.

AGU's Committee on the Structure of the Earth's Deep Interior (SEDI) is helping to coordinate mineral physics symposia at two conferences during the summer of 1989. A symposium on "Physics and Chemical Properties of the Deep Earth Materials" and a workshop on "Scientific Coordination of Research on the Dynamo Problem" will be held during the IAGA Workshop at the University of Exeter, U.K., July 19, 1989. Mineral physics will also be part of an SEDI symposium at the International Association for Seismology and Physics of the Earth's Interior meeting to be held in Istanbul, Turkey, August 30 to September 1, 1989. For more information, contact the mineral physics representative to SEDI, R. J. Hemley, Geophysical Laboratory, 2801 Upton Street N.W., Washington, DC 20008.

The International Mineralogical Association will hold its 15th General Meeting in Beijing, China, from June 28 to July 3, 1990. The IMA's Commission on Physics of Minerals will sponsor several symposia on theoretical and experimental mineral physics. Both contributed and invited papers will be presented. For more information, contact the Commission's Chairman G. David Price, Uni-

versity College London, Gower Street, London WC1E 6BT England, or the Secretary R. James Kirkpatrick, University of Illinois, Geology Department, Urbana, IL 61801.

The Department of Geological Sciences of the Virginia Polytechnic Institute and State University, Blacksburg, Va., will sponsor a meeting on research opportunities in mineralogy and mineral physics to celebrate the 70th birthday and illustrious career of F. Donald Bloss. The conference will be held in Blacksburg, Va., July 22–25, 1990. For more information, contact G. V. Gibbs, Department of Geological Sciences, VPI and SU, Blacksburg, VA 24061–0796.

### **GRL Call for Mineral Physics Papers**

The editors of Geophysical Research Letters are attempting to increase submission rates in the fields of solid Earth geophysics, and in particular, in mineral physics. GRL, which is noted for its record of rapid publication, welcomes short, original articles of new results presented in a way that will make their significance apparent to the general geophysics community. Manuscripts should be sent to a regional editor nearest you. Consult a recent issue for addresses.

### Call for Mineral Physics News and Announcements

"Mineral Physics News" appears biannually in Eos. News, notes, reviews, or other material of general interest to AGU and the mineral physics community are welcome. Please send information to the editor of Mineral Physics News.

### Mineral Physics Chairman's Corner



William A. Bassett, Chairman of the Mineral Physics Committee, shown with a petrographic microscope.

The Mineral Physics Committee is now in its fifth year. At the AGU Spring Meeting I became the third Chairman of the Mineral Physics Committee. I took over the position from my very able predecessors, Orson Anderson and Murli Manghnani. Orson, as the first Chairman, has the very big task of launching mineral physics as an independent field of research and organizing those of us who are active in this area. Murli carried on this initiative and was very effective in further raising the awareness of mineral physics in the Earth sciences community. An important measure of their success is the many excellent mineral physics sessions at AGU and other

meetings and the outstanding mineral physics publications that have appeared.

On September 28–30, 1988, a workshop was held at the University of California, Los Angeles Conference Center, Lake Arrowhead, to revise and expend the 1985 mineral physics workshop report titled *Mineral Physics; Atomic to Global*. By the end of 3 days of hard work, the group had produced 23 review papers on a wide range of mineral physics research topics from the behavior of aqueous solutions to the metallization of hydrogen in the major planets. These are now being gathered under one cover as 23 chapters of a report to be published by AGU. As the convenor, Tom Ahrens not only did an excellent

job of gathering people who represent a a good balance of topics but also drove all of us to get our writing tasks completed. When this report is published, it will be an exceptionally good guide to research in mineral physics, what has been accomplished, and what potentials exist for future work. We hope that this report will be useful in keeping members of the mineral physics community informed of activities in mineral physics, in helping members of sister disciplines know how they might interact with mineral physics, to inform people in management positions who help support mineral physics research, and to attract prospective young scientists into the field.

Elsewhere in this issue, you will find an an-

nouncement of the Mineral Physics award to pay the way each year for a promising student to attend AGU meetings. Won't you please support this award by contributing to the award fund and by suggesting the names of deserving students.

I look forward to the remaining year and half of my tenure as Chairman of this young field of research in the Earth sciences and will do all I can to help it to continue to

This item was contributed by William A. Bassett, Department of Geological Sciences, Cornell University, Ithaca, N.Y.