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FEATURE ARTICLE

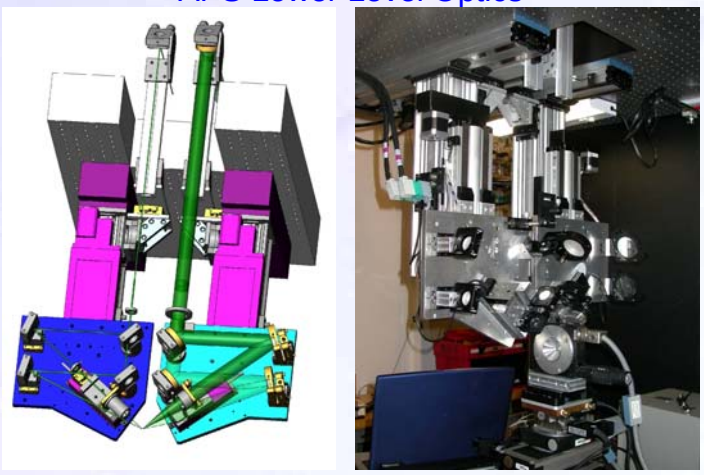
Brillouin Spectroscopy with Synchrotron Radiation at GSECARS, Advanced Photon Source

This article describes a project to design and install a Brillouin spectrometer, for measurement of sound velocities, on a synchrotron beamline at the Advanced Photon Source (APS). As discussed below, the combination of Brillouin scattering and X-ray diffraction can be a uniquely powerful tool for studies of the Earth's deep interior, and for improving the accuracy of high pressure experiments in general. This project has been undertaken as part of the COMPRES Infrastructure Development program, and the Elasticity Grand Challenge collaborative project supported by the Geophysics Program of the National Science Foundation EAR Division.

— Jay D Bass[1], Stanislav V Sinogeikin[1], Vitali B Prakapenka[2], and Guoyin Shen[2,3]

[1] *Geology Dept, University of Illinois, Urbana-Champaign, Urbana IL 61801*
jaybass@uiuc.edu
[2] *GSECARS, University of Chicago, Chicago IL*
[3] *Now at: HPCAT, Sector 16 APS*

Brillouin system at 13-BM-D GSECARS
APS Lower Level Optics



Over the past several decades, Brillouin scattering has become established as one of the main experimental techniques for measuring the elastic properties of Earth materials. With an even longer history of Earth science applications, x-ray diffraction (XRD) on samples compressed in a high-pressure apparatus (usually the diamond anvil cell, or DAC) can be used to measure the density of samples at high pressure and/or temperature, thereby allowing one to determine the P-V-T equation of state. These two types of experimental results are distinct but highly complementary, in that their combined results can yield a more complete description of the equation of state and thermodynamic properties of a material. In addition, the combination of these techniques allows the determination of absolute pressure scales, which is among the most pressing technical needs of the high-pressure research community.

Why Brillouin?: In a Brillouin scattering experiment, acoustic velocities Vp and Vs are measured on a sam-

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In this issue

-ple. These velocities are comparable with seismic velocities at depth in the Earth, thus allowing inferences about basic properties of the interior such as composition and temperature. Part of the attractiveness of this technique is that it is optical, thus making it possible to work with extremely small samples. In principle, any sample larger than a focused laser beam (5-10 μm) is suitable. In practice, we have worked with samples as small as 7 μm thick and less than 50 μm across. This makes it possible to work with small single-crystal or polycrystalline samples of high-pressure mantle phases, for example like $MgSiO_3$ perovskite. It also makes it possible to perform sound velocity measurements on samples at high pressure in a diamond cell, and/or at high temperatures. From a Brillouin scattering experiments we can obtain the adiabatic single-crystal elastic moduli, Cij, and the adiabatic bulk modulus (Ks) and shear modulus (G), as well as the velocities Vp and Vs for an isotropic polycrystalline aggregate.

Why Brillouin Scattering with X-rays? : The combination of these techniques allows velocities and Ks (by Brillouin), and the volume or density (by XRD) to be measured simultaneously. In high pressure experiments, synchrotron XRD is typically used to determine the P-V equation of state, and the isothermal bulk modulus $K_T = -V (\delta P/\delta V)$ (using a pressure standard such as ruby in the sample chamber). However, Brillouin scattering allows the bulk modulus to be measured independently through the elastic wave velocities: $K_S = \rho(V_P^2 - 4/3V_S^2)$. As first pointed out by Ruoff et al. (1973), since the bulk modulus is known from acoustic (Brillouin) measurements, knowledge of the volume from XRD allows one to determine the pressure P (with suitable conversion of Ks to K_T). Therefore, through the combination of Brillouin with XRD we can determine a primary pressure scale, that is independent of any other standards. The geophysical importance of defining accurate pressure scales was forcefully made by Irifune et al (1998), who found that the spinel-postspinel+MgO transition in Mg_2SiO_4 occurred at too low a pressure to explain 660 km seismic discontinuity. The determination of accurate primary pressure standards has since been recognized as one of the most important technical goals of the mineral physics community, and has been a high priority for COMPRES. A recent review of the issue has been presented by Fei *et al*. (2004). Complementary to the Brillouin-APS effort described here, are measurements being carried out using ultrasonics in the multi-anvil press and synchrotron radiation (Muller et al., 2003; Li et al., 2005). Multiple approaches to this problem will be needed and are one of the main objectives of the Elasticity Grand Challenge. The Brillouin scattering technique presently offers the best chance for determining primary pressure scales into the Mbar (100 GPa) region (Zha et al., 2000). Up till now, Brillouin spectroscopy has been done in a few highly specialized labs. An additional motivation for having a Brillouin spectrometer in a centralized facility such as the APS, was to make it more widely available to the entire mineral physics community.

<u>Description of the Brillouin-APS system.</u>

The new Brillouin system has been installed at GeoSoilEnviroCARS (GSECARS), sector 13-BMD of the APS. A number of special considerations had to be taken into account in building a Brillouin system on a beamline. Some of the main challenges were: 1) there is limited space; 2) the system must not interfere with other experiments performed at the beamline; 3) It must be possible to operate the system from outside the X-ray hutch. The design that was ultimately decided on is schematically illustrated in Fig. 1. A vertical scattering plane is used, in contrast to the horizon-

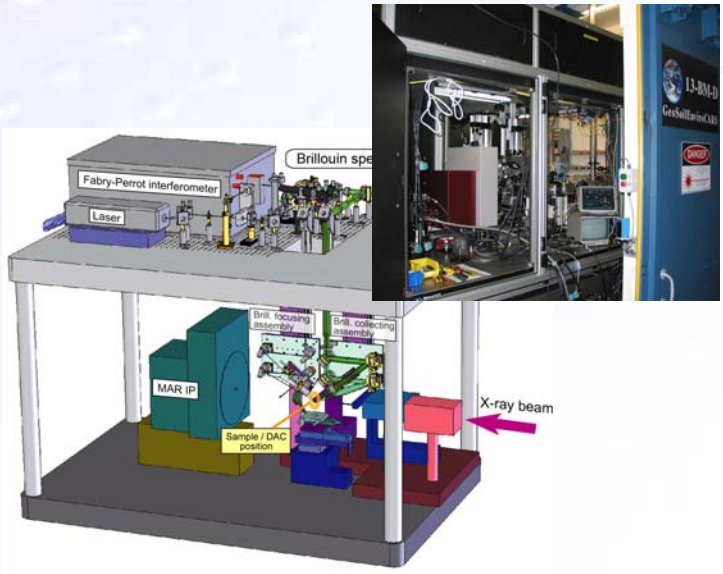

Fig.1 Schematic diagram of the Brillouin system at the APS. The lower level optics near the sample and X-ray beam are shown in an expanded view in the figure on page 1.

(continued on page 3)

tal configuration used in most labs, so that some of the optical components can be easily put into place and removed without interfering with other equipment. The scattered light collected from a sample in the X-ray beam is steered to an upper level several feet above where it is analyzed by a Sandercock-style 6-pass Fabry-Perot interferometer. The upper-level analysis optics are totally enclosed to comply with APS laser safety regulations. Figure 1 shows the lower level optics, which direct the probe laser (λ=532 nm) onto the the sample, and collect the scattered light with a 50° or 80° symmetric scattering geometry. A full description of the optical system is being submitted for publication (Sinogeikin et al., in prep.).

The First Data and Commissioning

Prototypes of the Brillouin system were built at the University of Illinois in 2002-2004. The system was moved to GSECARS and installed during 2004-2005, and the first data have been collected during two runs this year. Our first experiments this year were on MgO and NaCl, which are commonly used pressure markers (Fig. 2). Both single crystal samples (MgO and B1-phase of NaCl) and polycrystalline samples (B2 phase of NaCl) were examined at high pressures of about 30 GPa (for single crystals) and >70 GPa (for B2 NaCl). The quality of the Brillouin and X-ray data were excellent in all cases (Fig. 3).

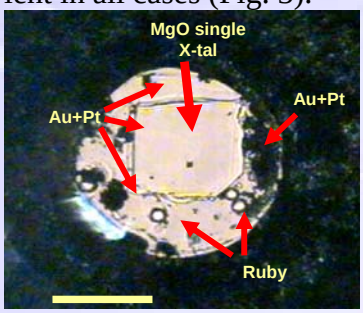

Fig. 2: Sample of MgO and several pressure markers loaded in the diamond cell for Brillouin scattering and X-ray studies at the APS. Scale bar is 100 microns.

In addition to experiments at room T, simultaneous high T and high P measurements were made using external resistance heaters. Laser heating using a CO_2 laser is planned for implementation at a later time.

Augmentation and additional refinements of the Brillouin system, to make it as user friendly as possible and to extend its capabilities, are being considered by COMPRES. In addition, the Infrastructure Development committee is considering supporting workshops to instruct potential users on the basics of Brillouin scattering and use of the facility.

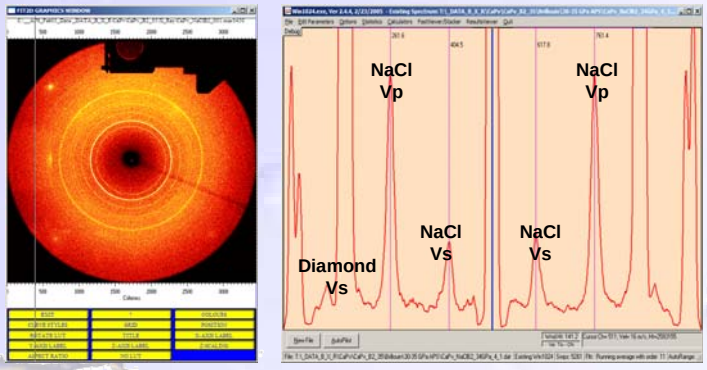

Fig. 3: X-ray (left) and Brillouin data for the B2 phase of NaCl at 35 GPa.

Acknowledgments: We acknowledge support of this project through a COMPRES Infrastructure Development subcontract (for equipment), and from NSF through the Elasticity Grand Challenge project (for personnel and related support). We also acknowledge GSECARS who provided partial support under their NSF and DOE contracts.

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President's Message

Bob Liebermann

We are proud of the awards and honors recently bestowed on members of the COMPRES community. These include:

At the AIRAPT Meeting in Karlsruhe, Germany in early July, Sergei Stishov received the Bridgman Medal for his pioneering research into the properties of materials at high pressures and temperatures.

On September 6, the International Balzan Foundation announced that its 2005 Balzan Prize in Mineral Physics is to be awarded to Russell J. Hemley and Ho-kwang (David) Mao of the Carnegie Institution of Washington. This prize carries a cash award of one million Swiss francs, half of which must be allocated to research projects involving young researchers. The award ceremony was held in Bern, Switzerland on November 11, 2005.

Frances Hellman, Professor at the University of California at Berkeley, has been selected to be the 2005 recipient of the Keithley Award of the American Phyical Society for her work in nanocalorimetry.

John Hall, a physicist at the National Institute of Standards and Technology [NIST] and the University of Colorado was one of the 2005 winners of the Nobel Prize in Physics. Dr. Hall has been collaborating with Ivan Getting on the Johnson noise thermometry project sponsored by COMPRES under the Infrastructure Development Program.

George Rossman of the California Institute of Technology has been awarded the 2005 Friedrich Becke Medal of the Austrian Mineralogical Society.

I attended a meeting the Science and Technology Steering Committee at the Brookhaven National Laboratory on July 14-15. One of the major agenda items were the evolving plans for NSLS-II which is now poised to receive Critical Decision -0 [CD-0 "Approve Mission Need"] from the Department of Energy, which would put it on the list of new construction projects, with an anticipated completion date of 2012. This CD-0 was approved by the Deputy Secretary of Energy on August 25, 2005.

COMPRES sponsored or co-sponsored a number of Workshops in the past four months:

On July 20-23, a VLab Workshop was held at the Minnesota Supercomputing Institute, convened by Renata Wentzcovitch. See http://www.vlab.msi.umn.edu/events/workshops.shtml for additional details and soon a report on the program.

On July 20-22, COMPRES sponsored a Workshop on High Pressure Melts, convened by Carl Agee and his colleagues. The participants of this Workshop are preparing a Grand Challenge collaborative research proposal to submit to the NSF Earth Sciences Division, perhaps in the CSEDI program.

On 21-23 October, a COMPRES-sponsored Workshop on "Rheology and Elasticity Studies at Ultra High Pressures and Temperatures" was

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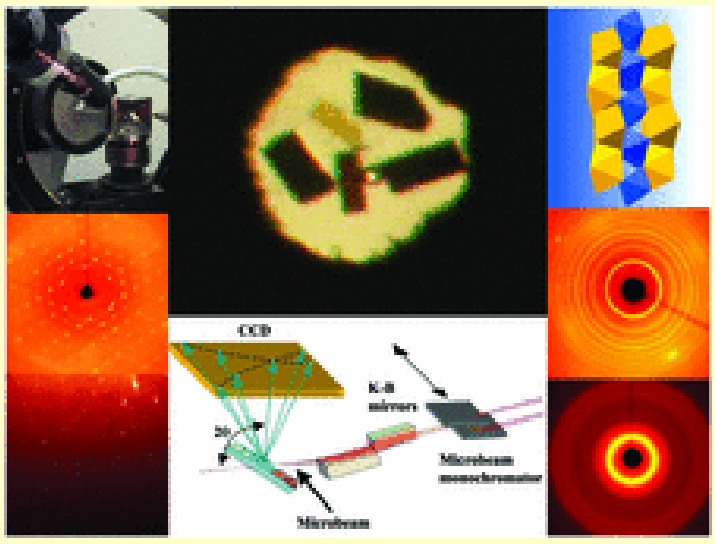

The *Journal of Synchrotron Radiation* published a special issue in September, 2005 devoted to single-crystal diffraction at high pressures. Composite image on the left (Cover of the special issue) shows various aspects of high-pressure XRD experiment: panoramic diamond anvil cell (DAC) used to generate pressure, sample in a DAC, composed of five magnesiowustite single crystals and a ruby sphere, polychromatic and monochromatic diffraction images from samples of different crystallinity ranging from single crystal to amorphous, experimental set-up for synchrotron polychromatic microdiffraction and example of crystal structure of a post-perovskite high-pressure phase.

President's message (*cont'd*)

held at HPCAT, APS, Argonne National Laboratory. Convened by Haozhe Liu of HPCAT, Rudy Wenk of the University of California-Berkeley, and Tom Duffy of Princeton University, the workshop attached more than 50 people who represented various parts of the deformation community. Two members of the Executive Committee [Harry Green and Don Weidner] were among the invited speakers and Mark Rivers and I attended as observers. Additional details may be found on the http://www.hpcat.aps.anl.gov/Hliu/Workshop/Index1.htm

Workshop on Evaluation of Synchrotron Mossbauer Data at the APS, October 290\-30, 2005. See details at: http://www.aps.anl.gov/News/Conferences/2005/Mossbauer_Data_Workshop/

"Synchrotron Infrared Spectroscopy for High Pressure Geoscience and Planetary Science" at NSLS, Brookhaven National Laboratory, November 3-5, 2005. See details at: http://www.nsls.bnl.gov/newsroom/events/workshops/ir/.

At the beginning of September, I attended the 3rd Workshop on Earth's Mantle Composition, Structure, and Phase Transitions" in Saint Malo, France from August 30-September 3. This COMPRES-sponsored Workshop was convened by Guillaume Fiquet, Jay Bass, Kei Hirose, and James Badro. More than 35 people attended, including many young scientists from Europe and a large contingent from Fei's lab at the Carnegie Institution of Washington. The scientific program was excellent, the site superb, the excursions well-planned and interesting, and the weather remarkable for this time of year in Brittany. See details of the program and associated activities at: http://deep.earth.free.fr/

While in France, I also visited the high-pressure beamline facilities at the European Synchrotron Radiation Facility [ESRF] in Grenoble and gave a seminar entitled: "Sound Velocities in Minerals under Mantle Conditions." My host was Wilson Crichton, Beamline Scientist on ID27. It was a special pleasure to see the wide range of high-pressure experiments being conducted on many different beamlines; see details at: http://www.esrf.fr/.

The team of Malcolm Nicol, Bonner Denton, Przemyslaw Dera, Robert Downs and Mark Rivers was awarded a Major Research Instrumentation grant by the NSF for "Development of Six New Approaches for Micro-focus Single-Crystal X-ray Diffraction for Materials Structure Research at Synchrotrons". This award is for three years with total funding of $720,000. This proposal was an outgrowth of a COMPRES-sponsored workshop organized by Przemek Dera and Charles Prewitt at the APS in November 2004.

On September 13, during the LANSCE Users Meeting at the Los Alamos National Laboratory, a half-day workshop was held on Neutrons at High Pressure. Keynote speakers included Yusheng Zhao of LANL on the conceptual design for a LAPTRON facility at LANSCE and Christopher Tulk of Oak Ridge National Laboratory on the design and progress of the SNAP project at the SNS, followed by discussion of the needs of users and tour of the high-pressure facilities at the Lujan Center.

The principal investigators in the Elasticity Grand Challenge collaborative research project held

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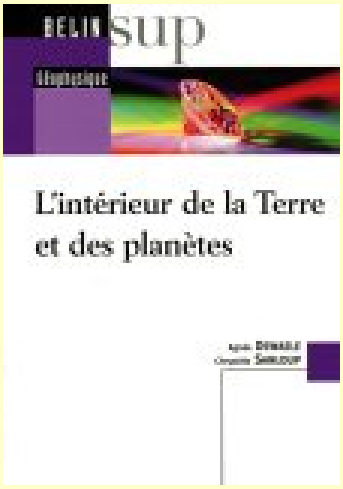

Interior of the Earth and planets: by Agnès Dewaele, and Christelle Sanloup

The Earth and planetary are very fascinating subjects. How geologists and geophysicists study their depths? How the Solar System can be simulated? Answers to such questions can be found in this book. It describes tools used by researchers to perform experiments in laboratory under extreme conditions; pressures and temperatures existing in the Earth and other planetary. Then, from recent and accurate data, the book proposes a summary of our understanding about mantle and core of the Earth as well as about the inner structure of the Giant Planets and their satellites.
http://dewaelea.free.fr/PageWeb1.htm

President's message (*cont'd*)

a working group meeting on Sept 17-18, 2005 at Stony Brook University. Convened by Jay Bass of the University of Illinois at Urbana-Champaign, this meeting was attended by G. Gwanmesia of Delaware State University, L. Stixrude of the University of Michigan, R. Wentzcovitch of the University of Minnesota, and B. Li, L. Li, M. Vaughan, D. Weidner and Liping Wang of Stony Brook University. I attended as an observer from COMPRES. As many of you will recall, there were four Grand Challenge initiatives submitted to the NSF contemporaneous with the COMPRES core proposal in August 2001; three of these were funded by EAR and have been an important scientific compliment to the COMPRES programs to support beamline operations at national facilities and nurture infrastructure development projects.

In the special election to fill the vacant position of Vice Chair of the Executive Committee, 36 of the 44 eligible U. S. member institutions submitted ballots. Quentin Williams was elected by a majority of those casting ballots, and will serve as Vice Chair of the Executive Committee until the end of his current term on the Executive Committee in June 2007. Quentin will also serve as the Secretary of the Executive Committee, continuing the tradition initiated by Shun Karato when he served as Vice Chair.

COMPRES coordinated and convened a "High Pressure Summit Meeting" on Sept 24-25, 2005 on Long Island, New York. This meeting is being held at the suggestion of David Lambert of the NSF-EAR and Nicholas Woodward of DOE-BES. Attendees include representatives COMPRES [H. Green, N. Ross, R. Liebermann], GSECARS [M. Rivers, S. Sutton], NSLS High Pressure Teams [D. Weidner, R. Hemley, M. Rivers, H-k. Mao], HPCAT [H-k. Mao], SNAP [C. Tulk, J. Parise, R. Hemley, H-k Mao] ALS-High P Partners [S. Clark, J. Zaug, H. Green], CDAC [R. Hemley], LANSCE [Y. Zhao], and CHESS [D. Bilderback]. The attendees are currently preparing a report which they will present to the program managers of the NSF and DOE in Washington on November 29, 2005.

A feature article written by me for EOS on behalf of the Executive Committee and the COMPREScommunity appeared in the 4 October 2005 issue [Vol. 86, No 40, pp. 365, 373]. You can download a pdf version of this article using the link on the COMPRES Home Page at http://www.compres.stonybrook.edu/Publications/RCL%20EOS%20MS/Published_article.pdf

On 14 October 2005, I attended the CARS Board of Governors meeting at the Advanced Photon Source as the new representative of GeoSoilEnvironCARS. A report on the review of the GSECARS operations was one of the features of the meeting, in which the close collaborative relationship between COMPRES and GSECARS was highlighted.

On 17-19 October at the GSA Annual Meeting in Salt Lake City, a Special Topical Session on High Pressure Mineral Physics was convened by William Bassett, Russell Hemley and Anne Hofmeister. This session was co-sponsored

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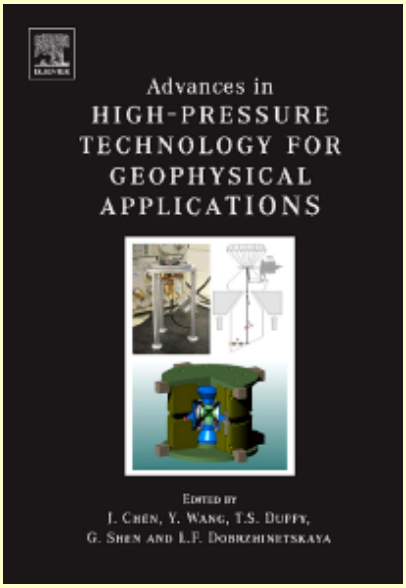


Advances in High-Pressure Technology for Geophysical Applications: by J. Chen, Y. Wang, T. S. Duffy, G. Shen, L. F. Dobrzhinetskaya

Over the past decade, some of the main developments in high-pressure technology focused on integration of analytical techniques with high-pressure apparatus, and pressure cell modifications for enlarging sample volumes and generating controlled stress fields. The technological frontiers are moving rapidly as the high-pressure community has expanded its access to large-scale radiation (synchrotron and neutron) sources worldwide. The exciting new developments in the high-pressure field have drawn growing attention from scientists in geophysics and other fields. This volume contains details of selected recent developments and will serve as a technical reference and handbook for both graduate or advanced undergraduate students as well as more senior researchers interested in keeping abreast of these new developments.

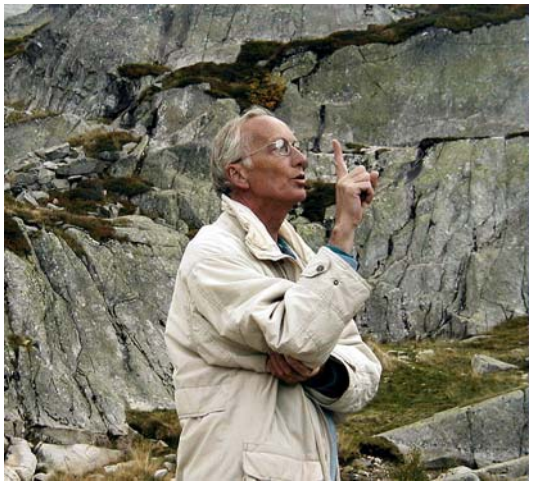
http://www.elsevier.com/wps/find/bookdescription.cws_home/705584/description#description

President's message (*cont'd*)

by the Mineralogical Society of America, Geophysical Laboratory of the Carnegie Institution of Washington and COMPRES. It celebrated Ho-Kwang Mao's receipt of the 2005 Roebling Medal and covered a broad spectrum of research in mineral physics.

On 20-21 October, I visited the Department of Geology and Geophysics at the University of Minnesota and gave a seminar entitled: "Sound Velocities in Minerals under Mantle Conditions." My host was David Kohlstedt, and I had the opportunity to visit the experimental laboratories of Kohlstedt and Mark Zimmerman [rock deformation], Marc Hirschmann [experimental petrology], and Subir Banerjee [rock magnetism].

The Facilities Committee of COMPRES paid a site visit to the GSECARS sectors at the APS on Oct 23-24, 2005. Charles Prewitt organized and chaired the visit, inasmuch as Mark Rivers is one of the two Project Managers/PIs of GSECARS; William Durham, Thomas Duffy and Abby Kavner all attended. Green and Liebermann attended as observers. The visit included talks by Rivers, Yanbin Wang, Vitali Prakapenka, and Steve Sutton, as well as a tour of the Sector 13 beamlines [both bending magnet and insertion device stations]. This visit also included a presentation with Guoyin Shen, now Project Manager of HPCAT and a visit to the Sector 3 beamline [hosted by Wolfgang Sturhahn] at which COMPRES is partially funding a postdoc to provide access to the nuclear resonant inelastic X-ray scattering facilities.



Olivier Jaoul (1944- 2005)

We are saddened to report that Olivier Jaoul of the Université Paul Sabatier in Toulouse, France died on November 15. Born in Neuilly sur Seine in 1944 and trained as a physicist in the laboratory of Jacques Friedel, Jaoul was recruited into geophysics by Claude Froidevaux at the Laboratoire de Géophysique et Géodynamique Interne at the Université Paris Sud in Orsay. In 1997, he moved his laboratory to Toulouse and joined the Laboratoire d'etude des Mécanismes et Tranferts en Géologie. In both Orsay and Toulouse, the Jaoul laboratory pioneered new experimental techniques to study plastic deformation and atomic diffusion in mantle minerals; this research was always characterized by care in design and execution of the experiments. The acquisition of new data for atomic diffusion led Jaoul and his colleagues to formulate a new model for creep of olivine via multi-component diffusion. Olivier was a master teacher, both at the undergraduate and graduate levels, with a refined pedagogical style which was both didactic and philosophical, typical of a person whose first foreign language was Greek. He enjoyed teaching young students, not only in the laboratory, but in the field, as can be seen in the photos here from a field trip to the Pyrenées with the first-year graduate students from Toulouse. Lastly, Olivier was a warm and generous colleague who leaves a long list of protégés and collaborators who are part of his scientific and educational legacy. He is survived by his wife Martine, and their two children, Nicolas and Delphine.

Photos taken at Lac d"Artouste in the Pyrenées, September 2002.

Recent PhDs

Heather Watson
Ph.D. 2005

Rensselear Polytechnic Institute

Dissertation: **Diffusion of siderophile elements in FeNi alloys, with applications to iron meteorites**

The process of diffusion is very important in many areas of Earth science. It is generally thought of as being "rate limiting" for many common processes such as crystal growth, and partitioning of elements. Because of this trait, concentration profiles emplaced through diffusive processes carry information regarding the thermal history of the object in question, including the cooling rates, timing and temperature of different phases throughout the object's history.

Several series of high pressure and high temperature experiments aimed at understanding the diffusive behaviour of siderophile (iron loving) elements and phosphorus at conditions that may be relevant to core formation, and to iron meteorites were performed. The model presented uses the experimental diffusion data to constrain the cooling rates of iron meteorites, and potentially give information about sizes of the cooling planetesimals , and the thermal state of the early solar system during their formation. Piston cylinder experiments at 1 GPa and 1100°C-1400°C revealed Arrhenius relations for Au, Pd, Cu, Re, Mo, and P. It was seen that the diffusivities of these elements span over an order of magnitude at the same conditions, which is a beneficial feature in helping to determine thermal histories. Multi-anvil experiments at 10GPa and 1100°C-1600°C also yielded Arrhenius relations for Au, Pd, and Re, and it was seen that there is a strong pressure effect on diffusion of these elements, although their relative diffusivities remain constant. A study of pressure dependence on diffusion of Au, Pd, and Re at 1400°C and pressures from 1 - ~25 GPa and P at 1300°C from 1-5 GPa activation volumes, including pressure dependent activation volumes for Pd and Au. The diffusivities of these siderophile elements show a possible linear dependence on ionic radius in the metal. P behaves quite differently than the other elements studied. It's diffusivity tends to be about 3 orders of magnitude higher than the other elements, it has a lower activation energy at 1GPa, and a much weaker dependence on pressure than Au, Pd, and Re. P is inferred to diffuse via an interstitial mechanism, as opposed to lattice diffusion.

The results from the 1GPa experiments have important applications in meteoritics. A finite difference model is developed with which siderophile element and Ni concentration profiles can be simulated in two phases of FeNi alloy undergoing slow cooling to form the characteristic Widmanstatten texture seen in iron meteorites. Matching many simulated profiles to observed profiles in natural samples, can give tighter constraints on the estimation of meteorite parent body cooling rates, and in turn, their sizes. A technique is described, using laser ablation ICP-MS, by which siderophile element profiles can be measured in taenite lamellae of meteorites with the appropriate spatial resolution and detection limits necessary to be used effectively with the model. The higher pressure experiments have implications for the limited mobility of siderophile elements in solid FeNi alloys such as planetary cores.

Statement: *I had a great experience as a graduate student working with Bruce Watson (Rensselear Polytechnic Institute) where I was first introduced to high-pressure experimental work on the piston cylinder apparatus, as well many other experimental and diffusion modeling techniques. This type of research certainly caught my interest, and I was fortunate enough to have an opportunity to visit the Geophysical lab as a pre-doctoral fellow where I could expand the pressure range of the experiments contributing to my dissertation. I am currently a post-doctoral fellow at the Geophysical Lab (Carnegie Institution of Washington) working with Yingwei Fei as a member of the Multi-anvil group. My present research interests include noble gas/trace element solubility in metallic liquids, and H solubility in lower mantle minerals (Al-perovskite). I am also continuing work on diffusion in metals at high temperature and pressure, and applications to iron meteorites.*

—Heather Watson

COMPRES Sponsored Workshop

Calorimetry on a Chip Workshop at COMPRES Annual Meeting June 16-19, 2005

The "Calorimetry on a Chip" workshop was held during the 2005 COMPRES annual meeting at Mohonk Mountain House - New Paltz, NY to present the capabilities and opportunities of the methodology and to discuss applications to mineral physics and a path forward. Alex Navrotsky and Frances Hellman made the presentation for about an hour total. It was followed by about 45 minutes of general discussion. The presentation will be available on the COMPRES website.

Major conclusions

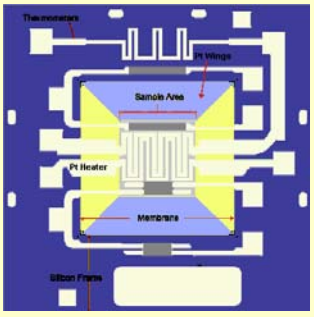
1. Calorimetry on a chip can measure heat capacities and detect and measure enthalpies of phase transitions at 4-500 K in samples under 1 mg in size. The main applications have been in magnetic thin films and some exploratory and proof of concept work needs to be done for powders and chunks of high pressure material. The method is potentially compatible with both multianvil and DAC experiments.
2. An exciting applications is to screen high pressure minerals for low temperature structural and magnetic transitions, especially in iron-bearing minerals Members of the scientific community could send or come with high pressure samples for such ex situ characterization. The systematics of how magnetic transitions depend on the structure of high P minerals will provide both fundamental physical and geophycally relevant new information
3. The combination of heat capacity and phase transition measurement can provide standard entropies of high pressure phases. The best attainable accuracy needs to be determined9 probably on the order of 1-3% in Cp).
4. The enthalpies of decomposition of high pressure phases might be measurable on small samples. If the decomposition product is well defined, this will provide ΔH of formation based on sub milligram and maybe microgram samples With (3) above one might get both ΔH and ΔS and thus ΔG based on small samples, and then calculate high P phase equiliabria.
5. The mineral physics community will gain experience with the chip fabrication technology which is familiar to the physics and materials communities. It will become feasible to design and mass produce other chip-based detectors for in situ high pressure work, including, but by no means limited to, calorimetry. This may be a major additional benefit of the calorimetry on a chip project.

The Path Forward

1. Between July and October of 2005, Navrotsky and Hellman and their groups including Maria Dorogova, a postdoc at Davis, will explore calorimetry on a chip for Fe_2SiO_4 olivine (fayalite) and its spinel polymorph. The former will be benchmarked against adiabatic Cp measurements, the latter represents new unexplored territory. Both Abby Kavner and Joe Smith have offered to provide samples.
2. Kavner, Hellman and Navrotsky will get together this summer to brainstorm on high pressure applications of chip technology and to tour the Microfabrication Lab at Berkeley.
3. Hellman will develop a plan for making her equipment and its software more user friendly and will think about what is needed to more easily accommodate visitors.
4. A proposal to COMPRES in November will include further exploratory experimental work and a possible workshop on the more general topic of "Mineral Physics on a Chip". Other larger proposals for the possible new science are anticipated.

— Alex Navrotsky

Calorimetry on a Chip



- **Weigh sample**
- **Weigh device**
- **Dab silver paint onto back of device**
- **Press sample into device and left to dry**
- **Weigh Device + Paint + Sample**
- **Mount device to frame**
- **Wire bonded pads to leads (thin Au wire)**
- **Measure heat capacity from ~2 K > 100 K**

Rheology and Elasticity Studies at Ultra-High Pressures and Temperatures

One of the major goals of geophysical research is to understand deformation in the deep earth. The COMPRES workshop on "Rheology and Elasticity Studies at Ultra-High Pressures and Temperatures" held on Oct 21-23, 2005 at APS, Argonne National Laboratory, has provided a great opportunity to assemble more than 50 geoscientists, experts in diamond anvil cell (DAC) design, structural refinement, and rheology, beamline scientists, postdocs and students from 6 countries, to define the current state of radial diffraction technology and research in ultra-high pressure deformation studies, push the technological frontier of deformation experiments in opposed anvil cells.

The workshop was divided into three sessions and there were 19 oral presentations. Bill Bassett and Dave Mao, pioneers in DAC radial x-ray diffraction studies, offered historic and current status review lectures at beginning of this workshop, and described the remaining technical challenges. These were followed by Sébastien Merkel's presentation on the recent results obtained from DAC radial diffraction and their applicability to Earth science. The keynote speakers from the deformation community presented important lectures on future directions: Harry Green led the discussions on opportunities and difficulties for rheological studies in the DAC; Takehiko Yagi delivered an excellent evening lecture (against the final game of the baseball World Series) on the radial x-ray diffraction studies in the DAC and Drickamer cell.

http://www.hpcat.aps.anl.gov/Hliu/Workshop/Index1.htm

Shun Karato offered the comprehensive introduction on the challenge for deformation studies in which mechanisms depend in a complex way on stress, strain rate, pressure, temperature, grain size and hydration state and recent high-pressure experimental studies on plastic deformation *via* rotational Drickamer cell. Don Weidner discussed stress measurements *via* D-DIA and the problems of elasticity studies under high P-T conditions in the plasticity dominated zone. Other speakers such as Agnès Dewaele showed new cutting-edge developments for high-pressure single crystal elasticity studies in the DAC up to 100 GPa; Robert Dinnebier demonstrated the advanced x-ray diffraction data analysis package to handle huge amount of high-pressure image plate data. Many other interesting and exciting talks were offered by distinguished experts in this field followed by fruitful discussions, and some conclusions for current status and future development needs were reached.

The panoramic DAC design, x-ray transparent gasket technology and advanced data processing methods have now been refined to the point where the radial DAC technique, such as quantitative Rietveld texture analysis, can be made available to a wider group of users. But several challenges need to be overcome in developing geophysically meaningful deformation experiments. New technological development efforts that will open new avenues for high-pressure rheological studies by the COMPRES community include development of new motor-driven panoramic diamond anvils cells for fine pressure and strain rate control, gasket technology optimization for high P-T radial diffraction, and development of a rotational laser heating system. Other important areas for development include the rotational DAC, high-pressure single crystal techniques and submicrometer x-ray application etc.

Although still in their infancy, radial x-ray diffraction techniques have provided important insights areas such as yield strengths at high pressure, and deformation behavior and texture development under compression. However, much further development is needed before we can achieve "real" rheological studies of geological materials under deep Earth conditions. The planned improvements to diamond cells, gaskets, and diffraction techniques, together with efforts to make radial diffraction more accessible to the COMPRES user community will set the stage for longer term developments and applications of the method, such as deformation studies of deep Earth materials at P-T conditions of the entire mantle and core.

This workshop provided an excellent environment in which the attendees including many students could learn from the balanced list of speakers who represented various parts of the deformation community. In the beamline experiment session, sample and gasket preparation procedures were shown. A sample of Fe at 81 GPa in a panoramic DAC was used to demonstrate radial x-ray diffraction. This was another important goal of this workshop: to provide hands-on training for students and postdoctoral researchers in this field so they can pursue new research directions.

— Haozhe Liu, Rudy Wenk, and Tom Duffy

Synchrotron Infrared Spectroscopy for High Pressure Geoscience and Planetary Science

Sponsored by COMPRES and the National Synchrotron Light Source (NSLS), the workshop on Synchrotron Infrared Spectroscopy for High Pressure Geoscience and Planetary Science was held at the NSLS on Nov. 3-5, 2005. The conveners were Zhenxian Liu and Russell J. Hemley. Thanks to the members of the COMPRES Executive Committee and the NSLS staff for suggesting, promoting, and supporting the IR workshop. It was a great success in terms of the excellence of the lectures, broad attendance that included many new potential users and student participation, extensive program, hands-on experiences for new users. More than 50 attendees took part (this was the maximum allowed by the budget and the size of the lecture room).

The workshop consisted of five sessions designed to accommodate the broad spectrum of attendees, ranging from experts to new users. The Friday morning session was directed toward attendees new to modern IR spectroscopy techniques in the field but it was also a very useful review of fundamentals and new developments for experienced users. Q. Williams (University of Califorinia Santa Cruz) gave a thorough overview on IR spectroscopy (and FT techniques in general) and its applications in the Earth sciences. G. Rossman (California Institute of Technology) gave a talk on hydrous components in the nominally anhydrous minerals, which was crucially important for users who are interested in the calibration of the water content in minerals. A. Hofmeister (Washington University in St. Louis) discussed the high pressure far-IR spectroscopy of mantle candidate minerals that are worth pursuing with the synchrotron technique. Finally, J. Tse (University of Saskatchewan, Canada) described theoretical methods for vibrational spectroscopy and many other applications.

The Friday afternoon session was started by L. Carr (NSLS, Brookhaven National Laboratory). He gave a very comprehensive talk on Fourier transform spectroscopy techniques using the synchrotron infrared source as well as an overview on the IR programs at the NSLS. There were seven additional speakers (A. Goncharov, V. Struzhkin, and S. Jacobsen, Geophysical Laboratory; D. Klug, Canadian Research Council; H. Scott, Indiana University South Bend; G. Lager, University of Louisville; and Y. Lee, Brookhaven National Laboratory) who discussed different topics related the works they have done at the U2A beamline. These talks not only addressed a broad range of problems in Earth and planetary sciences but also reflected new techniques developed at the U2A beamline in past years.

The third session, held Saturday morning, focused on imaging techniques combined with synchrotron sources. L. Miller (NSLS, Brookhaven National Laboratory) gave an extensive overview of chemical imaging at high spatial resolution using a synchrotron infrared microscope. Other speakers (L. Wang, SUNY; L. Dobrzhinetskaya, University of California Riverside; M. Koch-Müller, GeoForschungsZentrum Potsdam,

(continued on page 5)

Germany; and S. Clark, Advanced Light Source) gave talks featuring the applications of imaging techniques as well as high-pressure IR studies at other synchrotron sources. The facility tour and hands-on session on Saturday afternoon attracted more than 30 people. At the IR beamline, new users received detailed information on the beamline facility and its capabilities as well as first hand experience on how to perform high pressure IR experiments from the beginning to the end.

The last session for student/post-doc experiments at U2A beamline started right after the workshop. Two students and one post-doc submitted their research proposals and one day of beamtime was allocated per proposal. This new session offered not only a great opportunity to learn how to use the synchrotron IR facility but also a chance to collect valuable data for their research projects. The experiments went very well and the IR data they obtained are very interesting and will be publishable in scientific journals.

Finally, an open discussion brought a lot of attention to the future beamline developments. Liu and Hemley described the current status of the IR facility and its feasibility and abilities for general users as well as proposed beamline upgrades in the near future, such as combined laser heating and synchrotron IR spectroscopy for high pressure and high temperature experiments, new side station, imaging at ambient and high pressure, etc. The feedback from attendees has overall been very positive. There was great interest in adding laser heating capability. (IR workshop web site: http://www.nsls.bnl.gov/newsroom/events/workshops/ir/Default.htm).

— Zhenxian Liu

VLab tutorial on computational materials/mineral physics

The Virtual Laboratory for Earth and Planetary Materials, ***VLab***, (http://www.vlab.msi.umn.edu), the Minnesota Supercomputer Institute for Digital Technology and Advanced Computation, MSI, and the Italian National Simulation Center DEMOCRITOS (http://www.democritos.it/), announce a 2-week tutorial on first principles calculations. It will take place between May 21 and June 03, 2006, at the Minnesota Supercomputing Institute (MSI) at the University Of Minnesota, Minneapolis.

The first week will consist in presentations of the theoretical foundation. Whole day lectures intercalated by recitations. The second week will consist of hands-on experience with the open source (and free!!) package Quantum ESPRESSO (http://www.quantum-espresso.org). Whole day instructions and exercises on predetermined problems.

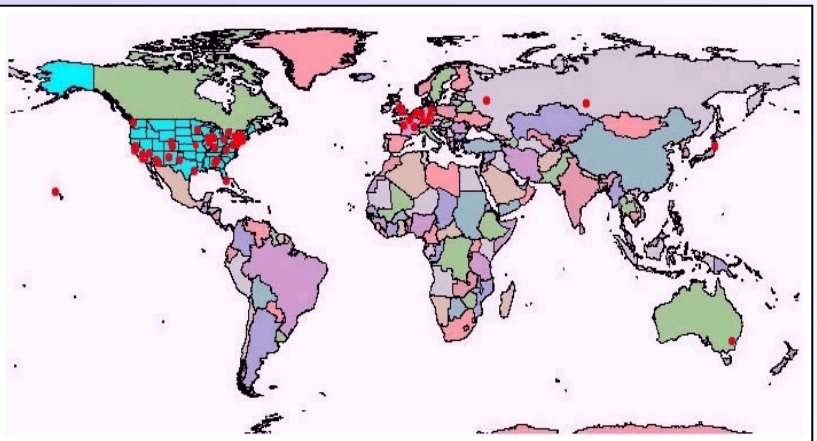
The syllabus will include some of these topics:
1st-2nd weeks: electron gas, Bloch functions and band structure, phonons, Hartree-Fock method, Density Functional Theory, exchange correlation functionals, pseudopotentials, density functional perturbation theory, molecular dynamics.
2nd week: Quantum ESPRESSO package, i.e., PWSCF, PHONON, plus auxiliary programs.

Confirmed instructors up to now: Dario Alfe' (UCL), Philip B. Allen (Stony Brook), Stefano Baroni (DEMOCRITOS & SISSA), Matteo Cococcioni (MIT/U of Minnesota), Stefano de Gironcoli (DEMOCRITOS & SISSA), Nicola Marzari (MIT), Ilja Siepmann (U of Minnesota), Don Truhlar (U of Minnesota), Renata Wentzcovitch (U of Minnesota).

The ***Vlab***, with the aid of MSI, will cover registration fee and will try to cover 100% of lodging and meals for all participants. The final level of financial support will be established after pre-registration deadline. Please write *asap* to Debbie Schutta (dschutta@msi.umn.edu) to pre-register and guarantee a spot. The number of participants will be limited. Pre-registration deadline is January 15, 2006.

COMPRES Annual Meeting, Membership

New Institutional Members



U. S. institutions: Los Alamos National Laboratory: Elector: Yusheng Zhao; Alternate: Neal Chestnut.
Foreign Affiliates: Vrije Universiteit in Amsterdam, The Netherlands. Representative: Wim van Westernen.
Australian National University, Australia. Representative: Hugh O'Neill.
Ehime University, Japan: Representative: Tetsuo Irifune
This brings the total of U. S. members to 45 and the number of foreign affiliates to 19.

2006 Annual Meeting

The Executive Committee of COMPRES has made a final decision on the dates and site for the 2006 Annual Meeting of COMPRES.

Dates:

Arrival: Tuesday, June 20, 2006 in afternoon or evening.

Departure: Friday, June 23, 2006 after lunch.

Site: Snowbird Ski and Summer Resort in Snowbird, Utah.

Located only 29 miles from Salt Lake City International Airport, with over 600 daily non-stop flights from most major U. S. cities. More information about the conference site is available at: http://www.snowbird.com/meetings/

These dates were specifically chosen to accommodate those persons who wish to attend the Gordon Research Conference on High Pressure at the University of New England [June 25-30, 2006]. We also hope to entice some of the GRC attendees and speakers to come early and join us at Snowbird.

Details of the program and registration/logistics will follow early in the new year. In the meantime, please send your suggestions for program content and format to

Robert.Liebermann@stonybrook.edu.

We encourage you to pencil these dates into your calendar at this time and look forward to seeing you at the Snowbird Ski and Summer Resort in June 2006.

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Rm 167, ESS Bldg. SUNY
Stony Brook, NY 11733
or +1 631 632 8213 or
alattimore@notes.cc.sunysb.edu

Feedback Slip (Fax to +1 631 632 8140)

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COMPRES Contacts:
President, Robert C. Liebermann, (631)632-1968, Robert.Liebermann@stonybrook.edu
Chair of Executive Committee, Harry Green, (951) 827-4505 (hgreen@mail.ucr.edu)
Administration, Ann Lattimore, (631)632-8213, alattimore@notes.cc.sunysb.edu
Newsletter Editor, Jiuhua Chen, (631)632-8058, Jiuhua.Chen@sunysb.edu