Earth Probe Newsletter
COMPRES
An NSF funded Consortium for Materials Properties Research in Earth Sciences
http://www.compres.us
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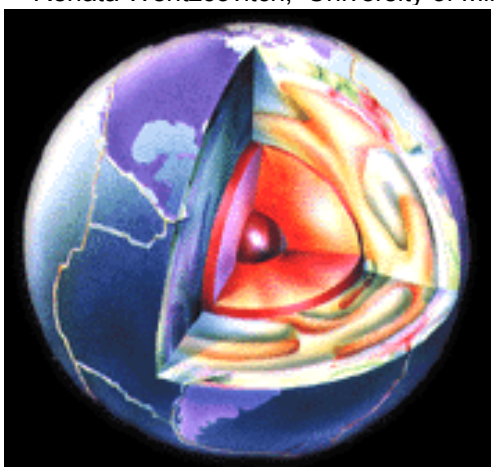
SPECIAL FEATURE

Virtual Laboratory for Earth and Planetary Materials, *VLab*

Renata Wentzcovitch, University of Minnesota

The pace of discoveries in Earth and planetary sciences has recently accelerated by large efforts such as the seismology consortia IRIS and Earthscope and by the mineral physics consortium COMPRES. NASA missions such as Cassini, that has reached Saturn this year, and will probe its icy Moon Titan in early 2005, and the Mars Exploration Rovers will accelerate further the pace of discoveries in this field. Observations collected by these projects and missions need to be backed up by reliable information on key planetary materials to be fully interpreted in the context of planetary processes.

This consortium was formed to promote developments in theoretical and computational Earth and planetary materials science. Experiments at planetary interior conditions are extremely challenging or virtually impossible. Theory may provide today and for a long time to come, the only way to obtain key information on materials properties at relevant conditions. The promotion of this field will be accomplished through the creation of a **Virtual Laboratory for Earth and Planetary Materials**, ***VLab***.



The ***Vlab*** is an interdisciplinary consortium that will **1)** address materials science problems related to planetary physics, **2)** use currently available methodologies and develop new ones to address these problems, **3)** explore emergent information technology resources to create novel human/software interfaces that will transform the way researchers interact with simulation techniques. This is urgently needed to empower also the non-specialist Earth and planetary sciences communities by enabling access and widening the use of the developing realistic and predictive materials simulation methodologies. The ***VLab*** will eventually turn into a public facility for the mineral physics community. It will also **4)** have educational and outreach programs to provide training and bridge the gap a) between mineral physicists and materials theorists and b) between under-represented groups in the sciences and the materials sciences and planetary sciences communities.

*The **VLab** is funded by NSF. Participating Institutions include: University of Minnesota, Stony Brook University, Information Technology, Louisiana State University, and UC-Santa Barbara. The first VLab workshop in Minneapolis will take place on 7/20-23, 2005. Information will be available at http://www.vlab.msi.umn.edu/.*

In this issue

President's Message

Bob Liebermann

COMPRES has now entered its third year. Since November 2002, we have been publishing quarterly Newsletters to inform the COMPRES and broader communities of the current activities of COMPRES as an organization and high-pressure mineral physics as a scientific discipline. These have been edited by Jiuhua Chen, Associate Director of the Mineral Physics Institute of Stony Brook University. The Executive Committee of COMPRES has concluded after the first two years of these quarterly newsletters that they are an important and effective means of communication and have decided to continue publishing the Newsletter, but at a reduced frequency of every three months. It is our intention to publish new issues of the COMPRES Newsletter each February, June and October; this issue for March 2005 is slightly delayed due to other priorities.

Following are some of the highlights of activities of the COMPRES and related scientific communities during the period October 2004 to February 2005.

Workshop on "Structure Determination by Single Crystal X-ray Diffraction (SXD) at Megabar Pressures". This workshop was organized by Przemyslaw Dera and Charles T. Prewitt and held at the Advanced Photon Source of the Argonne National Laboratory on November 13-14, 2004. Harry Green and Nancy Ross represented the COMPRES committees at this workshop. A separate report on this workshop appears elsewhere in this newsletter and additional details may be found on the COMPRES website at: http://www.compres.stonybrook.edu/Workshops/Structure%20Determination%20at%20a%20Megabar/sxd_meeting_report.pdf

As a consequence of the revision of the COMPRES ByLaws by vote of the Electorate [September 29, 2004], the President is no longer a member of the Executive Committee. In an election held in November 2004, Quentin Williams of the University of California at Santa Cruz was elected to be a member of the Executive Committee and will serve a term from December 2004 to June 2007 (the unexpired term of the President).

We are especially pleased to congratulate Dave Mao on his recent double honors in being selected for two presitgious awards: (1) The Roebling Medal of the Mineralogical Society of America; and (2)The Gregori Aminoff Prize in Crystallography from the Royal Swedish Academy of Sciences

I spent two weeks at the Australian National University in Canberra, conducting a collaborative research project with Professor Ian Jackson in October and November. During these visits, I also gave a seminar on the topic of:"Sound Velocity Measurements in Mantle Minerals under Mantle Conditions".

COMPRES and its community had a major presence at the Fall 2004 Meeting of the American Geophysics Union in San Franscisco last December. See separate report elsewhere in this newsletter for details.

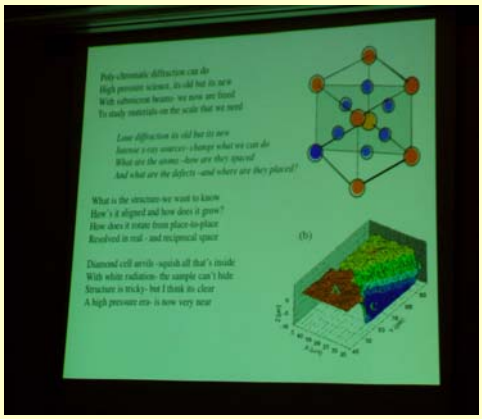
On January 2005, the American Geophysical Union announced the election of 43 new Fellows

(*continued on page 3*)

"Polychromatic microdiffraction"

Poly-chromatic diffraction can do
High pressure science, its old but its new
With submicron beams- we now are freed
To study materials-on the scale that we need

Laue diffraction its old but its new
Intense x-ray sources- change what we can do
What are the atoms –how are they spaced
And what are the defects –and where are they placed?



What is the structure-we want to know
How's it aligned and how does it grow?
How does it rotate from place-to-place
Resolved in real - and reciprocal space

Diamond cell anvils -squish all that's inside
With white radiation- the sample can't hide
Structure is tricky- but I think its clear
A high pressure era- is now very near

Presented by Dr. Gene Ice at the Workshop on ***Structure Determination by Single Crystal X-ray Diffraction (SXD) at Megabar Pressures***

President's message (*cont'd*)

and Medalists. On behalf of the mineral and rock physics and chemistry communities, COMPRES can point with pride to the members of its extended community who will be honored this year, including:

New AGU Fellows:

Bruce Buffett, University of Chicago
Reid Cooper, Brown University
Geoffrey David Price, University College London
David Yuen, University of Minnesota
Vladimir Zharkov, Institute of Physics of the Earth, Moscow

Macelwane Medal: Paul Asimow, California Institute of Technology

Hess Medal: Sean Solomon, Carnegie Institution of Washington

Lehmann Medal: Thomas Jordan, University of Southern California

Our heartiest congratulations to those to be honored in 2005.

The Science Advisory Committee (SAC) of the National Synchrotron Light Source at the Brookhaven National Laboratory is in the process of reviewing all of the operations of the NSLS. To prepare for this review, subpanels were established to review subsets of the NSLS beamlines, including those beamlines operated and maintained by members of the COMPRES community with funding from the NSF via COMPRES. These high-pressure beamlines include the Diamond-Anvil Cell facilities at X17B3 and X17C and U2A [H-k. Mao and R. J. Hemley of the Carnegie Institution of Washington] and the Multi-Anvil Facilities at X17B2 [D. J. Weidner, Stony Brook University]. I represented COMPRES and its Executive Committee. Mark Rivers represented the University of Chicago and GSECARS, which will assume responsibility for the management of the DAC facilities on May 1, 2005.

COMPRES' Annual Report for Year #3 [May 2004 to April 2005] and the Annual Program Plan and Budget for Year #4 [May 2005 to April 2006] was submitted to the NSF on February 3, 2005. The full Year #3 Annual Report can be viewed on the COMPRES website at the new url: www.compres.us. This report was approved by David Lambert, the cognizant Program Director for COMPRES at the NSF on February 4, 2005.

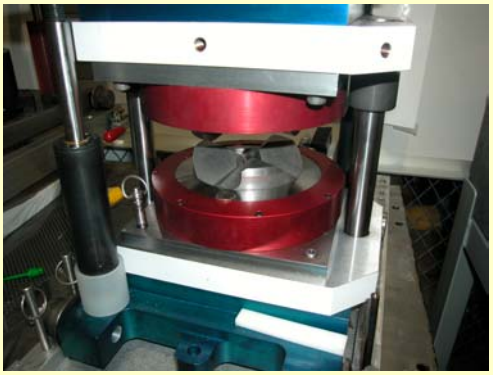
Alexandra Navrotsky of the University of California has been selected to be the recipient of the 2005 Harold Urey Medal of the European Association of Geochemistry. This medal will be presente to Alex at the annual Goldschmidt meeting in Moscow, Idaho, in May 2005.

On Friday, February 11, I visited the APS to discuss progress and plans at several of the beamlines, including:

Large-volume facilities at GSECARS—Y. Wang and N. Nishiyama
Laser-heating infrastructure development project—A.Campbell and G. Shen
DAC facilities at GSECARS—G. Shen and V. Prakapenka
Brillouin spectrometer infrastructure development project—J. Bass, D. Lakshtanov and G. Shen
HPCAT—D. Haussermann

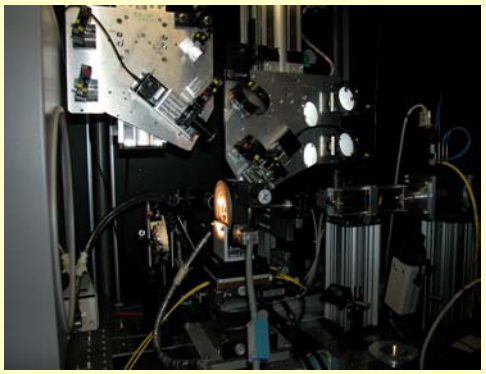
(*continued on page 4*)

Photos from Bob's APS visit



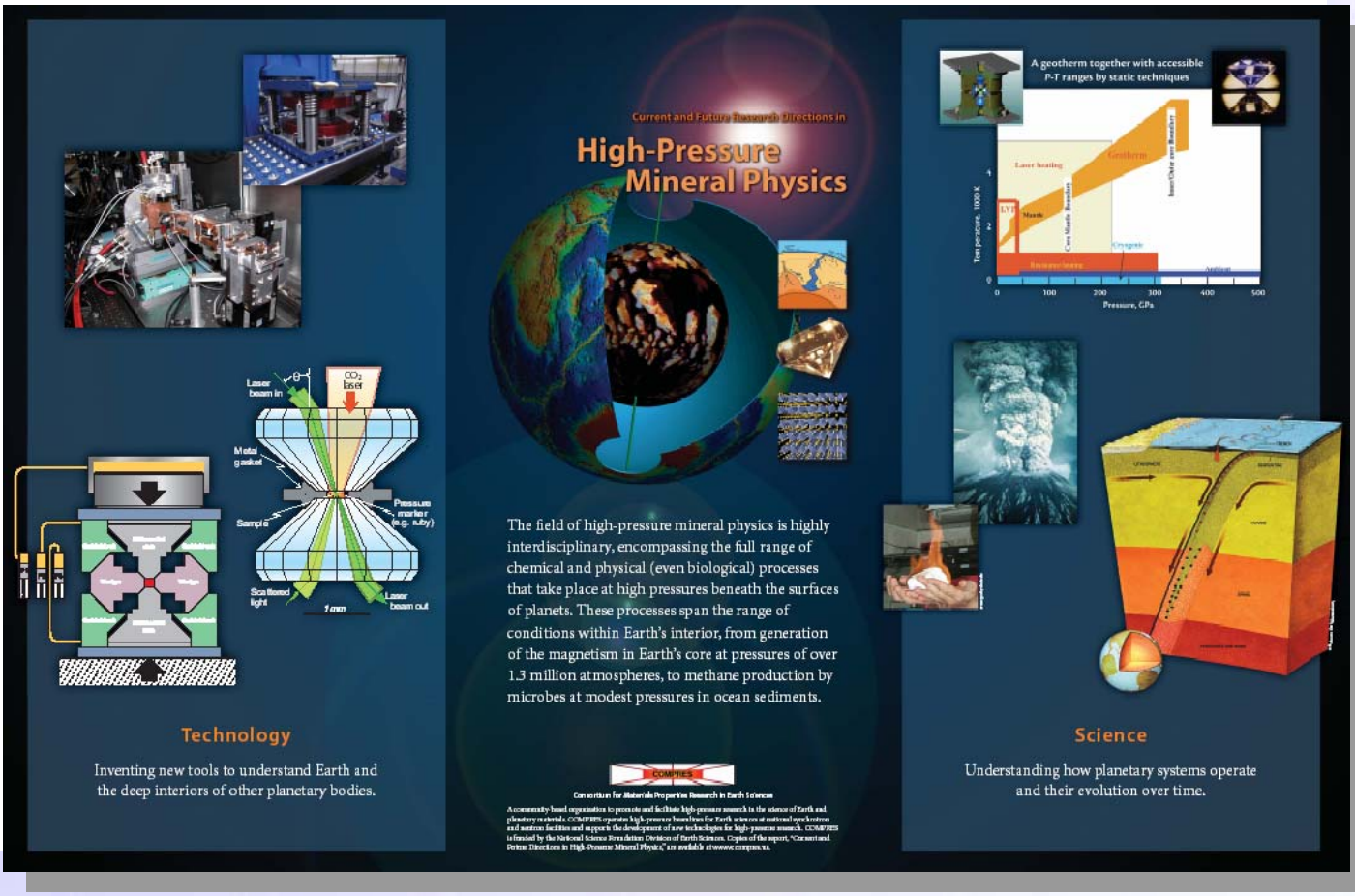
T-10 apparatus of Kawai-type

Controlpanel for high P Brillouin experiments



"Insides" of Brillouin spectrometer

Bass Report Poster



A poster based on the COMPRES Bass Report "Current and Future Directions of Research in High-Pressure Mineral Physics" has been designed in collaboration with Ellen Kappel of GeoProse for general public outreach. An electronic copy of the poster is available for downloaded at the Publications page of the COMPRES website (http://www.compres.us). Full-size copies at 24" x 36" of this poster will be available at the 2005 Annual Meeting.

President's message (*cont'd*)

While at the APS, I also attended the Workshop on Nuclear Resonant Scattering on Earth Materials using Synchrotron Radiation on February 11-13, organized and convened by Wolfgang Sturhahn, Jay Bass and Michael Lerche. A report on this Workshop appears elsewhere in this newsletter.

In consultation with the Executive Committee, we prepared a one-page PowerPoint slide for David Lambert at NSF-EAR to use in presentations within the NSF. A copy may be viewed elsewhere in this newsletter and may also be downloaded from the Publications page of the COMPRES website.

In collaboration with Ellen Kappel of GeoProse, we have designed a poster based on the report on "Current and Future Directions of Research in High-Pressure Mineral Physics", the so-called Bass Report. A copy may be viewed elsewhere in this newsletter and may also be downloaded from the Publications page of the COMPRES website. Full-size copies at 24" x 36" of this poster will be available at the 2005 Annual Meeting at Mohonk Mountain House, June 16-19, 2005 [see details in special article on the meeting in this newsletter].

COMPRES 4th Annual Meeting

Mohonk Mountain House, New Paltz, NY, June 16-19, 2005

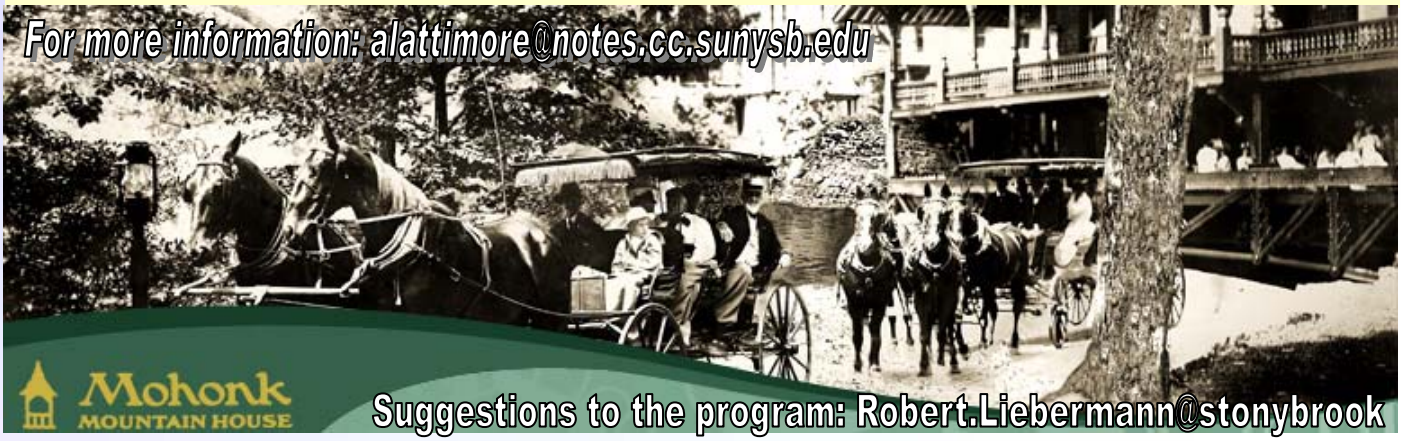
- *Scientific presentations*
- *technological presentations*
- *group discussions*
- *annual business meeting*

- Members of the COMPRES community will be offered:
  - double-room accommodation
  - all meals for the duration of the meeting [starting with dinner on Thursday, June 16 and finishing with lunch on Sunday, June 19].
- Additional details and costs for accompanying persons may be found on the Registration site.
- COMPRES will be unable to cover travel expenses for attendees.

Travel Scholarship:

Travel scholarships will provide full or partial travel scholarships to those graduate students presenting abstracts for poster presentations at the Annual Meeting. The scholarships include up to $500 each for travel expenses incurred in attending the Annual Meeting; reimbursement will be via travel vouchers submitted with receipts at or following the meeting. To be eligible for a travel scholarship, the graduate student must do the following:

1. **Apply for consideration for a travel scholarship via email to Ann Lattimore [alattimore@notes.cc.sunysb.edu] by May 20, 2005. This application should include the following:**
   - **(a) Cover page indicating the name, address, telephone number, FAX number and email address of graduate student, and the name and address of the mentor/advisor.**
   - **(b) Abstract including title and authors, with the applicant as the presenter.**
   - **(c) A paragraph by the applicant describing where they are in their graduate studies and why they want to attend the Annual Meeting.**
2. **A letter of recommendation from their mentor/advisor. This letter should also detail the group's travel funding and explain why the travel scholarship is needed for the student.**
3. **Submit an abstract for a poster presentation via the website. The abstract MUST be submitted for the application to be considered for approval and award of a travel scholarship.**
4. **Register for the Annual Meeting on the website**



COMPRES 3rd Annual Report Submitted to the NSF

In 2004, substantial progress has been made in achieving the objectives and goals of the Consortium for Materials Properties Research in Earth Sciences [COMPRES]. Major technological advances at the community facilities operated by COMPRES at national laboratories and the infrastructure development projects sponsored by COMPRES have enabled new scientific research opportunities in the field of high pressure mineral physics and chemistry.

The management of these community facilities and infrastructure development projects is monitored by Standing Committees elected by the representatives of the member institutions of COMPRES under policies and procedures established by the committees and endorsed by the Executive Committee. As the consequence of a membership campaign, there are now 41 U. S. institutions which are voting members of COMPRES [the Electorate] and another 16 non-voting institutions overseas which have affiliate membership.

COMPRES has sponsored and/or organized many workshops and scientific meetings in the past year. These include the COMPRES Third Annual Meeting in Lake Tahoe, California in June and working group meetings for the Grand Challenge teams in "Ultra-High Pressure Rheology" at Yale University in May 2004 and "Elasticity of Mantle Minerals" at the University of Illinois at Urbana-Champaign in May 2004. Other workshops: (1) "Future Directions for the Laser-Heated Diamond Anvil Cell at the Advanced Photon Source, at the Argonne National Laboratory in March 2004; (2) Focused Ion Beam (FIB) Applications in Earth Sciences at the University of California at Riverside in March 2004; (3) SCEC/COMPRES Workshop on the "Science, Status and Future Needs of Experimental Rock Deformation" at Mt Holyoke College in August 2004; and (4) Structure Determination by Single Crystal X-ray Diffraction (SXD) at Megabar Pressures at the Argonne National Laboratory in November 2004.

The process of reviewing and revising the ByLaws of COMPRES, initiated at the 2003 Annual Meeting in Santa Cruz, was completed in September 2004. The revised ByLaws are posted on the COMPRES website at: http://www.compres.stonybrook.edu/AboutUs/Bylaws/index.html.

In September, COMPRES announced the publication of a new report entitled: "Current and Future Research Directions in High-Pressure Mineral Physics." This report is an outgrowth of the discussions and results of a Workshop on "A Vision for High Pressure Earth and Planetary Sciences Research: The Planets from the Surface to the Center" which was held on March 22-23, 2003 in Miami, Florida. The NSF Division of Earth Sciences commissioned and supported this workshop, and COMPRES organized it. Fifty-five scientists attended the Workshop, which was convened by Jay Bass and Donald Weidner.

The Annual Report for Year #3 presents an overview of the activities of COMPRES, detailed reports from each of the Community Facilities operations and Infrastructure Development projects supported by COMPRES, the budget plan for Year #4 [May 1, 2005 to April 30, 2006]. The full Report can be viewed on the COMPRES website at the new url: www.compres.us

This report was approved by David Lambert, the cognizant Program Director for COMPRES at the NSF on February 4, 2005.

COMPRES at Fall AGU meeting 2004

- Exhibition booth jointly sponsored by GSECARS and COMPRES, which attracted lots of visitors, and which featured copies of the "Bass Report" on "Current and Future Research Directions in High Pressure Mineral Physics", as well as COMPRES calendars for 2005.
- The COMPRES Standing Committees held breakfast meetings to discuss the annual reports on the Infrastructure Development projects and Community Facilities. The Executive Committee met for breakfast on Dec 15 to begin the planning process leading to the submission of the Annual Report for Year #3 and Program Plan and Budget Request for Year #4 to the NSF on February 1, 2004.

COMPRES Sponsored Workshops

"Structure Determination by Single Crystal X-ray Diffraction (SXD) at Megabar Pressures"

Organizers:
Przemyslaw Dera, *Geophysical Laboratory, Carnegie Institution of Washington*
Charles T. Prewitt, *University of Arizona, Tucson*

In response to the proposal submitted last year to the Infrastructure Development Committee, COMPRES awarded us a budget of $20K to organize a workshop focused on the future of ultrahigh-pressure single-crystal XRD techniques, aimed at "building on the strengths of the existing high-pressure crystallographic community by bringing together the top experts from around the world to plan a coordinated way forward." This report summarizes the results of this successful two-day meeting, held on November 13-14, 2004, at the Argonne National Laboratory (Advanced Photon Source) in Chicago.

One of the main objectives of this workshop was to provide answers to the following questions:

a. Is it scientifically important/justifiable to develop megabar SXD techniques?
b. Is there enough interest and demand in the community for such development?
c. Is there a consensus among the experts on how such a task should be approached?
d. How can the effort be coordinated and managed most efficiently?

The meeting was very well attended, attracting over 60 participants, 14 of which came from outside US, representing 5 different countries. The high attendance of this relatively specialized workshop alone makes a strong case that there is indeed sufficient interest and demand in the community to develop high-pressure single-crystal techniques at the various synchrotron radiation sources. Our highly focused workshop was timed at a critical juncture in the early development of Mbar single-crystal techniques, and brought together nearly all the active experts and a wide range of supporters representing complementary specialties (such as microdiffraction). A full report of the workshop can be found at: http://www.compres.us/Workshops/Structure%20Determination%20at%20a%20Megabar/sxd_meeting_report.pdf

"Nuclear Resonant Scattering on Earth Materials using Synchrotron Radiation"

On February 11-13, a workshop on Nuclear Resonant Scattering on Earth Materials using Synchrotron Radiation was organized at Advanced Photon Source (APS) of Argonne National Laboratory by W. Sturhahn of APS, G. Shen of University of Chicago , J. Bass and M. Lerche of University of Illinois at Urbana-Champaign. This workshop brought together more than 30 people, including experts in these techniques and new potential users from the COMPRES community. A full report will be available on the COMPRES website.

Recent PhDs

Couvy, Hélène Ph.D 2005

Bayerisches Geoinstitut, Universität Bayreuth (Germany)
and
Laboratoire de Structure et Propriétés de l'Etat Solide, Université des Sciences et Technologies de Lille (France)

Dissertation**: Experimental deformation of forsterite, wadsleyite and ringwoodite: Implications for the seismic anisotropy of the Earth's mantle**

The rheological properties of the major minerals of the Earth's mantle are still not well constrained. However, these properties are crucial for the understanding of a wide range of processes in the Earth's interior such as mantle convection. The purpose of this work is to address the issue of the rheology of the lowermost upper mantle and of the transition zone through the mechanical properties at high pressure of olivine (with forsterite composition Mg_2SiO_4) and of its high-pressure polymorphs wadsleyite and ringwoodite. Indeed, the properties of the Earth's mantle can be inferred as a first approximation from the mechanical properties of those polymorphs which volumetrically dominate the mineralogy of the region of concern.

Deformation experiments have been performed on hot-pressed forsterite samples and on pre-synthesized wadsleyite and ringwoodite samples under pressure conditions of the Earth's mantle and at 1300-1400°C. The possible influence of the phase transformation from forsterite to wadsleyite on rheology has been also investigated. Deformation has been achieved by shear using the Kawai-type multianvil apparatus. Complementary experiments on forsterite have been performed in the newly developed Deformation-DIA. Some of them have been carried out on a synchrotron beam line to perform *in-situ* stress and strain measurements. In order to gain a maximum of infor-mation on the defor-mation mechanisms and on the Crystallographic Preferred Orientation (CPO), a special attention has been devoted to the microstructural characterisation of the samples. Electron BackScattering Diffraction (ESBD) and Transmission Electron Microscope (TEM) have been mainly used.

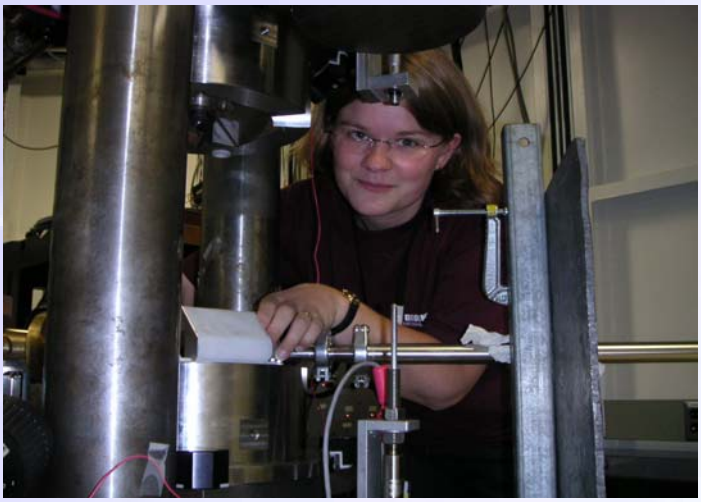


Photo taken at X17B2 of the NSLS

An important pressure-induced change in deformation mechanism is shown in forsterite. The deformation of forsterite at high pressure and temperature is dominated by the [001]{hk0} slip system rather than the [100](010) glide which is extensively observed at low pressure and high temperature..

Concerning the high-pressure polymorphs, their plastic behaviour has been studied with a strong emphasis on the formation of CPO. ViscoPlastic Self Consistent (VPSC) modelling is used to link the CPO with known elementary deformation mechanisms of these phases. The main features of the CPO of wadsleyite are characterized by the alignment of the [100] axes parallel to the shear direction and the alignment of the [001] axes toward the normal to the shear plane. Too many uncertainties remain on the ringwoodite CPO for them being used to interpret seismic anisotropy.

Finally, we suggest that strain-induced CPO might be responsible for the seismic anisotropy observed in the lowermost upper mantle and in the upper part of the transition zone. The low seismic anisotropy of the lowermost upper mantle can be explained from the slip system change in forsterite and the CPO of wadsleyite point toward a dominant tangential flow in the upper part of the transition zone.

"This PhD work has been co-directed by Prof. Patrick Cordier (LSPES, University of Lille) and Prof. Falko Langenhorst (BGI, University of Bayreuth). It was a great pleasure to work with them on the deformation of mineral under high pressure. I carry on working on this topic as post doc in MPI at Stony Brook" —— *Hélène Couvy*

From COMPRES Beamline Interns

Christopher Young

I received my Bachelor's degree in chemical engineering/materials science and engineering from UC Davis in June 2004. I served as an undergraduate research assistant at LLNL under the direction of Joe Zaug. At LLNL I studied the physical properties of high-explosives under extreme conditions in a diamond anvil cell. I also performed preliminary studies with the pressure induced band-gap transition of CdTe nanocrystalline semiconductors.

Now as the current intern for COMPRES at the NSLS I have the opportunity to explore an entirely new field. I have been working with Jiuhua Chen (SUNY-SB) and other visiting scientists on a variety of projects. The main focus has been on high pressure and high temperature melt properties, synchrotron capability development, and deformation experiments using the D-DIA. Below is a summary of the projects that I have been working on.

Density of Molten FeS:

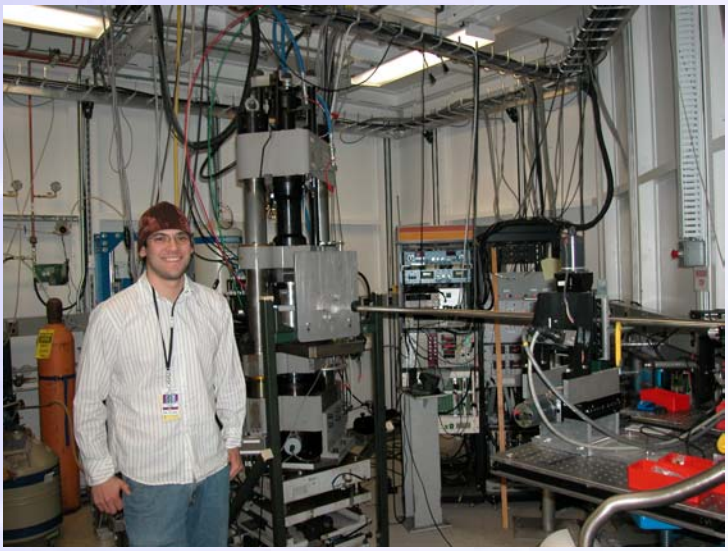
Studying the liquid properties of metals at earth core conditions has long been a difficult task. The SAM-85 large volume press at X-17B2 provides us the opportunity to study melt density at high pressure and temperature. The density measurements are made using an x-ray imaging plate. The density can be calculated using the radiograph intensity and known x-ray absorption properties of the absorbing metal. Using a modified Beer's law, accounting for spherical geometry, we find the density as follows with a constant x-position:

$$B(x_c, y) = Ce^{-[\mu_{FeS}\rho_{FeS}(D(x_c,y)-l(x_c,y))+\mu_{Al_2O_3}\rho_{Al_2O_3}l(x_c,y)]} \quad (1)$$

$$l(x_c, y) = 2[r^2 - (x - x_0)^2 - (y - y_0)^2]^{1/2} \quad (2)$$

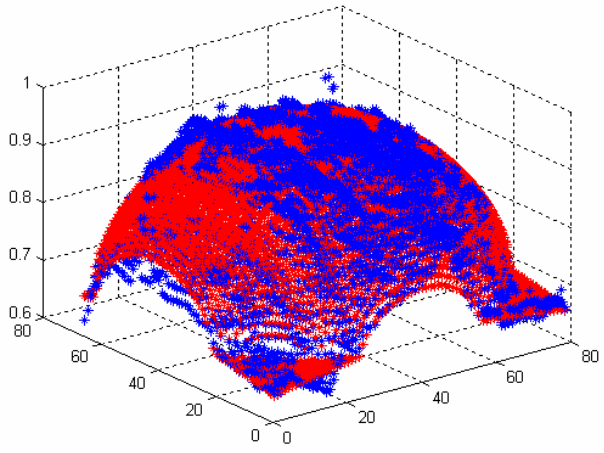
$$D(x_c, y) = (D_0^{\,2} - x^2)^{1/2} \quad (3)$$

Where μ is the mass absorption constant, ρ the density, I_0 the intensity of the entering x-ray, D_0 the diameter of the cylindrical sample chamber, r is the radius of the Al_2O_3 sphere, x and y are the coordinates of the pixels, x_0 and y_0 are the center coordinates of the Al_2O_3 sphere. Using two dimensional fitting provides an approximate result, however it is much more desirable to constrain the fitting to the entire image. A 3-D model for the intensity across the sphere is as follows:



$$B(x, y) = I(x, y)Ke^{-[\mu_{FeS}\rho_{FeS}(D(x,y)-l(x,y))+\mu_{Al_2O_3}\rho_{Al_2O_3}l(x,y)+\mu_0\rho_0 d_0]} \quad (4)$$

In equation 4, μ_0 ρ_0 d_0 is a correction factor for the absorption of the surrounding materials. Using a 3-D model to find the density of the molten FeS should provide a much more accurate result. The figure at the bottom is a representative image of the 3-D fitting that has been performed. The blue points are the experimental data and the red points represent the fitted points from the non-linear regression. A coauthored paper on molar melting volume of FeS at high pressure has been accepted for publication in *"Advances in High Pressure Technology for Geophysical Applications"* (Editors: J.Chen, Y. Wang, T.S. Duffy, G. Shen and L. Dobrzhinetskaya). Further revision to the code needs to be added to achieve a better fitting for the 3-D pattern.



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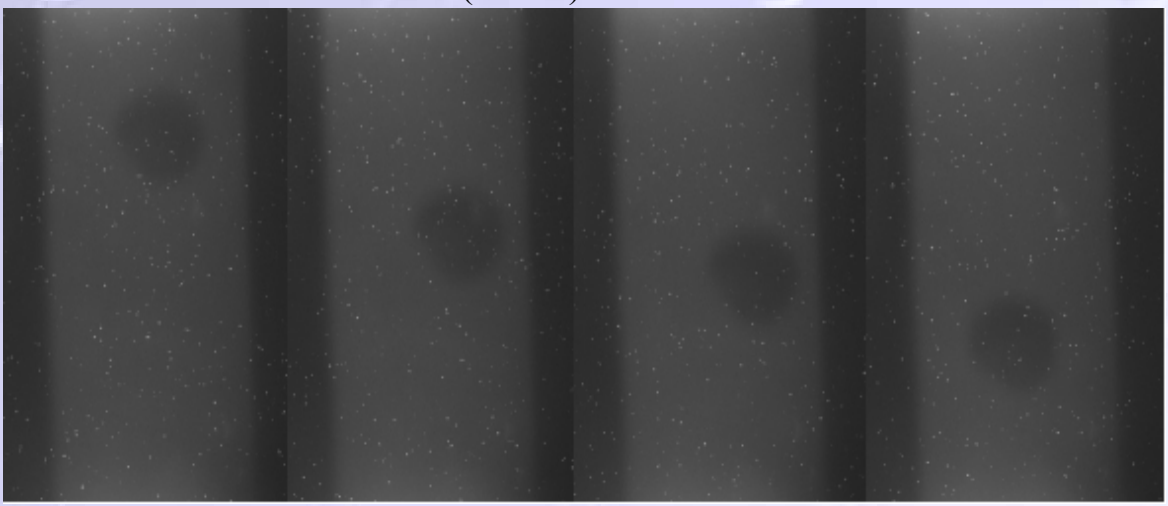
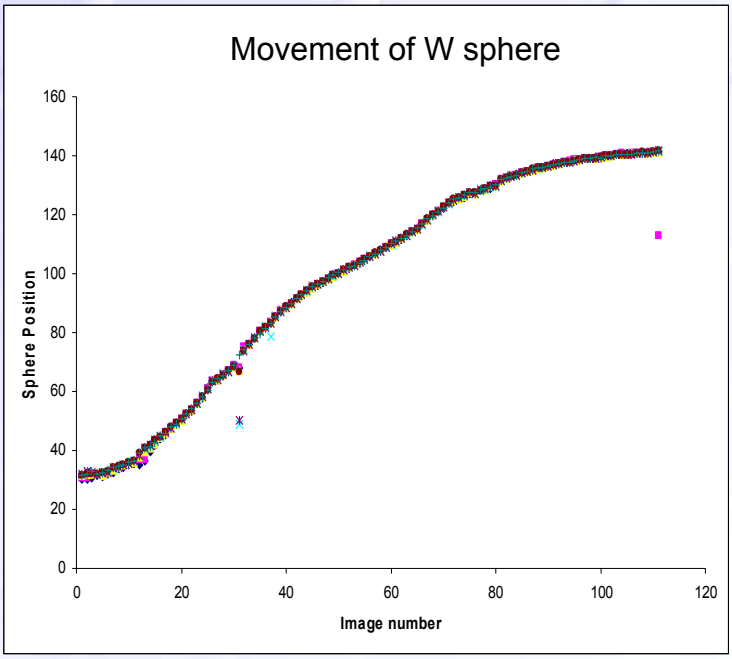
From COMPRES Beamline Interns (*cont'd*)



Viscosity of Sn:

X-ray radiography at X-17B2 also provides the opportunity to measure the viscosity of melts at high pressure and temperature. In these experiments a small W sphere is placed in a sample. As the temperature rises and the sample melts the W sphere will move vertically in the sample. The speed that the W sphere descends through the material can be tracked using the radiographs. The acceleration of the sphere can then be related to the viscosity of the material. As the viscosity of the material decreases the speed of the sphere will increase. The above figure shows the motion of a W sphere with time: Each image is taken over a specified time interval. These 4 images are only representative and are not spaced equally over tine. Figure on the right is a graph showing the motion of the sphere over a complete time series.



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