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Understanding Electronic Spin States of Iron in the Earth's Lower Mantle

— Jung-Fu Lin

This article describes recent research results on the nature and effects of the spin transition of iron in the Earth's deep mantle. These recent results are providing new aspects of our understanding of the geophysics and geochemistry of the Earth's interior.

Earth's lower mantle is the most voluminous layer of the Earth and consists of ~20% ferropericlase [(Mg,Fe)O] and ~80% silicate perovskite [Al-(Mg, Fe)SiO_3], in addition to a small amount of calcium silicate perovskite ($CaSiO_3$). Iron (Fe) is the most abundant 3*d* transition metal in the Earth's interior. The unique electronic oxidation and spin states of iron give rise to complex physical and chemical properties of the Earth's interior. With recent advances in high-pressure diamond anvil cell (DAC) techniques and synchrotron based X-ray facilities, pressure-induced electronic spin-pairing transitions of iron have been detected in the lower-mantle ferropericlase and silicate perovskite in high-pressure X-ray emission, Mössbauer, and X-ray diffraction experiments at lower-mantle pressures (e.g., Lin *et al*., 2005a,b; 2006a,b; 2007) (Fig. 1,2).

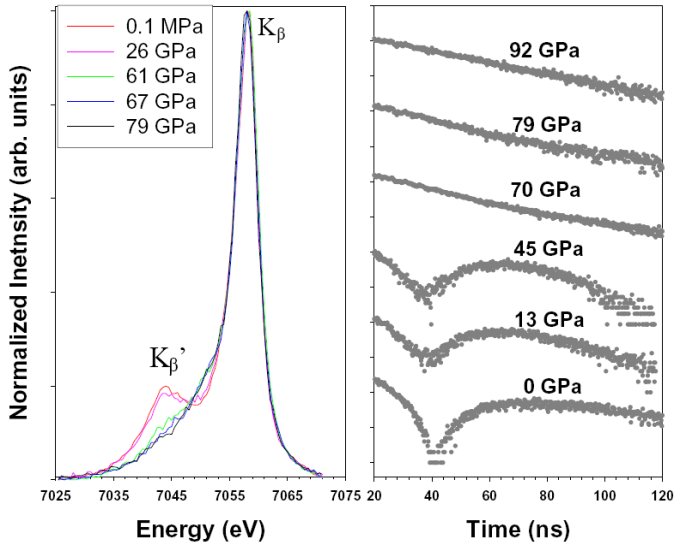

Figure 1. Experimental observations of the electronic spin-pairing transition of iron in ferropericlase [$(Mg_{0.75},Fe_{0.25})O$] under high pressures and room temperature. (*left*) Representative X-ray emission spectra of Fe-K_β collected from a single-crystal ferropericlase (Lin *et al*., 2005a). The presence of the satellite peak (K_β') at ambient pressure and 26 GPa is characteristic of the high-spin state of iron whereas the absence of the satellite peak above 61 GPa indicates the occurrence of the low-spin ferropericlase. (*right*) Representative synchrotron Mössbauer spectra of ferropericlase (Lin *et al*., 2006a). The quantum bits at 0, 13, and 45 GPa are generated from the quadrupole splitting of the high-spin state of iron in the sample, whereas the flat feature of the spectra at 70, 79, and 92 GPa indicates disappearance of the quadrupole splitting and the occurrence of the low-spin state.

Under ambient conditions, the ferrous iron in ferropericlase is in the high-spin state with four unpaired and two paired 3*d* electrons. The existence of the high-spin Fe^{2+} can be observed by the appearance of the satellite X-ray emission peak (K_β') located at the lower energy region of the main emission peak ($K_{\beta 1,3}$) of ~7058 eV, which results from the 3*p*-3*d* core-hole exchange interaction in the final state of the emission

(*continued on page 2*)

In this issue

FEATURE ARTICLE

process (Fig. 1). On the other hand, Fe^{2+} has all six 3*d* electrons paired in the low-spin state, which is characterized by the disappearance of the low energy satellite peak due to the loss of the 3*d* magnetic moment. Such high-spin to low-spin transition is also clearly detected in high-pressure synchrotron Mössbauer study of ferropericlase (Lin *et al*., 2006a) (Fig. 1); the appearance of the quadrupole splitting indicates the existence of the high-spin state of iron in the sample, whereas its disappearance signals the occurrence of the low-spin state. The spin transition of iron in the lower-mantle phases results mainly from the fact that the crystal field splitting energy increases with respect to the exchange splitting energy at high pressures, and it becomes energetically favorable for electrons to occupy orbitals with opposite spin in the low-spin state.

Understanding the effects of the spin transitions on the physical and chemical properties of ferropericlase and silicate perovskite at high pressures and temperatures is becoming critical in reliably evaluating the geophysical and geochemical implications of the spin transitions. An X-ray diffraction study of $(Mg_{0.83},Fe_{0.17})O$ to 135 GPa by Lin *et al*. (2005a) first revealed a dramatic increase in the isothermal bulk modulus (K_T) and bulk sound velocity (V_Φ) across the electronic spin-paring transition (Figure 2). It is perhaps surprising to note that such study was the first attempt to measure the compression behavior of the second most abundant lower-mantle phase to the pressures of the lowermost mantle. It is even more intriguing to envision that such local, tiny electronic transition may have profound geophysical implications in the most voluminous layer of the Earth's interior.

Recent high-pressure DAC study using nuclear resonant inelastic X-ray scattering spectroscopy at XOR-3 of the Advanced Photon Source further shows that compressional and shear wave velocities and their pressure derivatives rise dramatically across the spin-pairing transition of iron in $(Mg_{0.75}Fe_{0.25})O$ above 50 GPa (Lin *et al*., 2006b). The electronic spin-pairing transition of iron is also found to significantly influence other elastic, thermodynamic and vibrational properties of the iron component in $(Mg_{0.75},Fe_{0.25})O$ (Lin *et al*., 2006b).

The high-spin and low-spin states of Fe^{2+} in ferropericlase can be treated as two distinct phases with unique physical properties, though a mixed population of the high-spin and low-spin states, a spin crossover, is predicted to occur at lower-mantle pressures and temperatures. Although the nature of the electronic spin-pairing transition under high temperatures of the Earth's lower mantle has yet to be understood experimentally, recent theoretical predictions suggest that the transition in ferropericlase would occur over an extended pressure range of approximately 30 GPa (or ~700 km in depth) (Sturhahn *et al*., 2005; Tsuchiya *et al*., 2006). As such, the associated effects on the physical properties across a gradual spin crossover in ferropericlase (and perhaps in silicate perovskite and post perovskite) should be reduced. Such theoretical predictions are motivating experimental mineral physicists to directly measure the spin states of iron in oxides and silicates under the pressure-temperature conditions of the Earth's lower mantle.

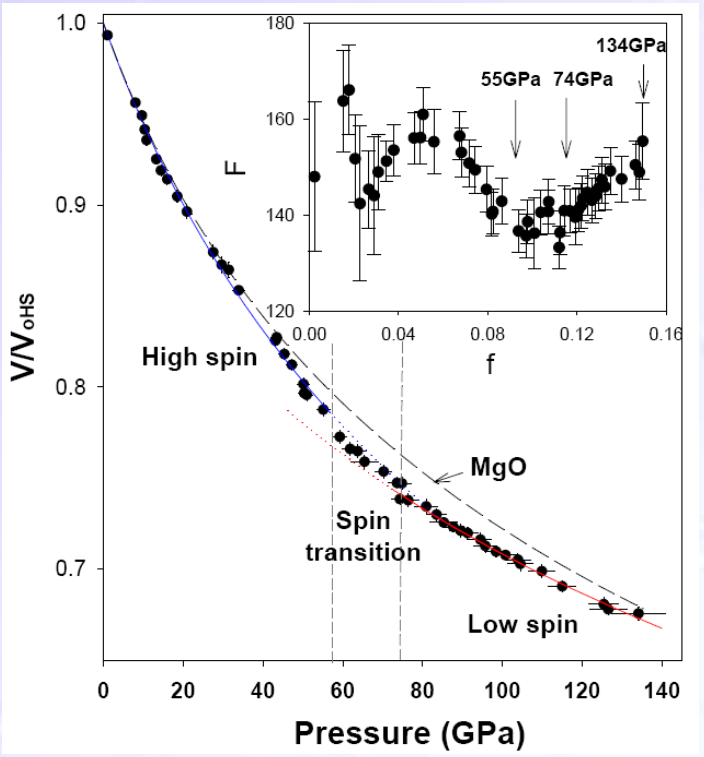

Figure 2. Normalized volume of ferropericlase-$(Mg_{0.83},Fe_{0.17})O$ as a function of pressure at 300 K (Lin *et al*., 2005a). Blue curve and red curve represent the compression behavior for the high-spin and low-spin states, respectively. V_{0HS} is the volume of the high-spin state at ambient conditions. Dash black line represents the compression curve of MgO. Insert, normalized stress (F) versus normalized strain (f) plot. F decreases with increasing f up to 55 GPa, whereas the F increases with increasing the f above 74 GPa, indicating a significant change in the incompressibility from the high-spin state to the low-spin state. A volume decrease can also be seen across the transition, although an accurate value for the volume reduction remains to be further determined.

(*continued on page 3*)

Electronic Spin States

(*cont'd*)

One approach for studying the electronic spin states and the crystal structures of the candidate mantle phases under high pressures and temperatures is to interface the X-ray emission spectroscopy and X-ray diffraction with the laser-heated diamond cell (Fig. 3) (Lin *et al*., 2005b). This pilot study points to the unique capability of the integrated techniques to address the issue of the electronic spin transition or crossover in 3*d* transition metals and compounds under extreme high pressure-temperature conditions. Such study also points to the need for other integrated facilities for the mineral physics community in order to tackle complex properties of candidate materials in the Earth's interior.

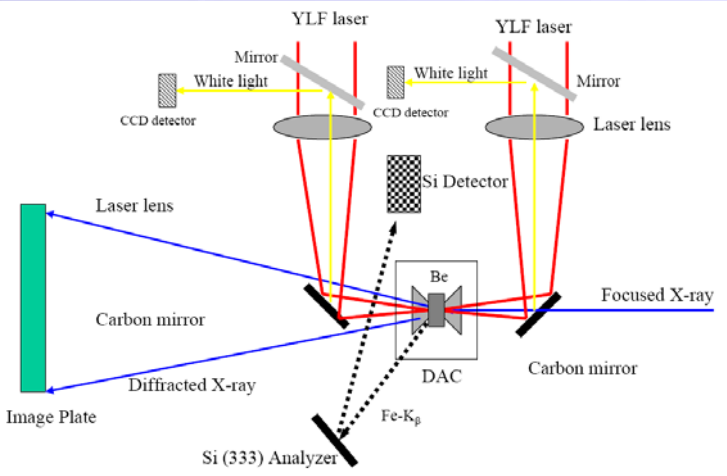

Figure 3. X-ray emission spectroscopy and X-ray diffraction with laser-heated diamond anvil cell experiments at the GSECARS of the Advanced Photon Source (Lin *et al*., 2005b). The system is constructed in order to study the spin states of iron in mantle oxides and silicates under high pressures and temperatures. The Fe-K_β fluorescence lines were collected through the Be gasket by an one-meter Rowland circle spectrometer in the vertical scattering geometry. An image plate (MAR345) was used to collect diffracted X-ray in the forward direction.

Although these recent results have revealed complex behavior of iron in oxides and silicates under high pressures and room temperature, many aspects of the nature of iron in the Earth's interior remain unknown (see Lin *et al*. (2007) for further discussions). Therefore, the ultimate goal in the study of mineral physics of the Earth's interior is to eventually measure the spin and oxidation states as well as physical properties of the candidate mantle phases under lower-mantle pressure-temperature conditions. Such goal requires future developments and integration in many synchrotron-based facilities as well as new frontier collaboration.

Acknowledgments

This article is derived from a series of collaboration projects conducted at HPCAT, GSECARS, XOR-3 of the APS and at the Geophysical Laboratory and Lawrence Livermore National Laboratory. These facilities are partially funded by the COMPRES program. This work at LLNL was performed under the auspices of the U.S. DOE by University of California and LLNL under Contract No. W-7405-Eng-48.

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Selected References:

1. Lin, J. F., V. V. Struzhkin, S. D. Jacobsen, M. Hu, P. Chow, J. Kung, H. Liu, H. K. Mao, and R. J. Hemley (2005a), Spin transition of iron in magnesiowüstite in Earth's lower mantle, *Nature*, **436**, 377-380.
2. Lin, J. F., V. V. Struzhkin, S. D. Jacobsen, G. Shen, V. Prakapenka, H. K. Mao, and R. J. Hemley (2005b), X-ray emission spectroscopy in a laser-heated diamond anvil cell: probing spin state of transition metals in the Earth's interior, *J. Synchrotron Rad.*, **12**, 637-641.
3. Sturhahn, W., J. M. Jackson, and J. F. Lin (2005), The spin state of iron in Earth's lower mantle minerals, *Geophys. Res. Lett.*, **32**, L12307, 10.1029/2005GL022802.
4. Lin, J. F., A. G. Gavriliuk, V. V. Struzhkin, S. D. Jacobsen, W. Sturhahn, M. Y. Hu, P. Chow, and C. S. Yoo (2006a), Pressure-induced electronic spin transition of iron in magnesiowüstite-(Mg,Fe)O, *Phys. Rev. B*, **73**, 113107.
5. Lin, J. F., S. D. Jacobsen, W. Sturhahn, J. M. Jackson, J. Zhao, and C. S. Yoo (2006b), Sound velocities of ferropericlase in Earth's lower mantle, *Geophys. Res. Lett.*, **33**, L22304, doi:10.1029/2006GL028099.
6. Tsuchiya, T., R. M. Wentzcovitch, C. R. S. da Silva, and S. de Gironcoli (2006), Spin transition in magnesiowüstite in Earth's lower mantle, *Phys. Rev. Lett.*, **96**, 198501.
7. Lin, J. F., S. D. Jacobsen, Renata M. Wentzcovitch (2007), Electronic spin transition of iron in the Earth's deep mantle, *Eos. Trans. AGU*, Vol 88, No 1, 13, 24.

President's Message

Bob Liebermann

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

Shun Karato of Yale University was selected to receive the 2006 Vening Meinesz Medal of the School of Geodynamics. Each year, the VMSG Medal is presented to a distinguished scientist, who has contributed very significantly to the field of geodynamics.

From the ETH in Zürich, Switzerland comes news of two major awards:
Artem Oganov received the Latsis Prize for signific contributions to mineral physics.
Colin Glass received the ETH Zürich medal for Outstanding Student Research Work.

At the Fall 2006 AGU Meeting in San Francisco we all took special pride in the award of honors and medals to our colleagues in Mineral and Rock Physics and related fields, including:

Dan Frost—James Macelwane Medal
Alexandra Navrotsky—Harry Hess Medal
Subir Banerjee—Fleming Medal
Bruce Watson—Bucher Medal

On Friday, October 6, I attended the semi-annual meeting of the CARS Board of Governors at the Advanced Photon Source of the Argonne National Laboratory, as one of the representatives of GSECARS; the other representative is Dion Heinz of the University of Chicago.

While at the APS, I took the opportunity to visit with people at the APS who are in working on projects supported by COMPRES. These included:

Vitali Prakapenka, Guoyin Shen, and Alexei Kuznetsov who are working on the development of a new CO2-laser heating system for DAC devices. This project is being conducted by a team led by Thomas Duffy at Princeton University, in collaboration with Dion Heinz at the University of Chicago and the others.

Mark Rivers on Johnson noise project, which was transferred from the University of Colorado to the University of Chicago in 2005; Yanbin Wang is now in charge of this project, in collaboration with Ivan Getting, but was in Japan at SPring-8.

Mark Rivers and Clayton Pullin on designs for new gas-loading system to be installed in one of the prep rooms within the GSECARS complex at the APS and be made available to all members of the COMPRES community.

Vitali Prakapenka on the Brillouin spectroscopy system developed by the team led by Jay Bass of the University of Illinois at Urbana-Champaign. It is now open for beamline applications from general users.

Wolfgang Sturhahn on the development of both nuclear resonant inelastic X-ray scattering and inelastic X-ray scattering at Sector 3. He also gave a tour of the new Sector 30 with its sumptuous setting and nice new facilities.

On October 9 and 10, I attended an external review of Machine Operations Reliability Evaluation

(*continued on page 5*)

Prof. Shun-ichiro Karato, Department of Geology and Geophysics, Yale University received the 2006 Vening Meinesz Medal of the School of Geodynamics. The VMSG Medal is installed to commemorate Prof. Dr. Ir. Felix Andries Vening Meinesz (1887 - 1966) and presented to a distinguished scientist, who has contributed very significantly to the field of geodynamics each year. Prof. Karato delivered his VMSG lecture at the 9th VMSG Symposium on November 1, 2006, Delft University of Technology, Aula.

President's message (*cont'd*)

(MORE) at the NSLS of Brookhaven National Laboratory. This review was commissioned by Chi-chang Kao, the new Chair of the NSLS (effective 1 October 2006), and was conducted by a distinguished panel with members from the Stanford Synchrotron Radiation Laboratory, the Advanced Photon Source at Argonne National Laboratory, the Synchrotron Radiation Center of the University of Wisconsin, and other departments at Brookhaven. I was invited by Kao to be an observer representing the Science and Technology Steering Committee of the Brookhaven Science Associates.

On October 19 and 20, I visited high-pressure experimental laboratories in Cambridge, Massachusetts, including:

> The shock-wave laboratory of Sarah Stewart-Mukhapadhyay at Harvard.
>
> The diamond-anvil cell laboratory of Dan Shim at MIT.

On October 20-21, I attended a Symposium in Honor of Professor Brian Evans at MIT. This event was held to celebrated Brian's 60th birthday and drew speakers from around the world who presented papers on Earth Materials—Deformation and Transport Properties; many of the speakers were former graduate students or postdoctoral mentees of Brian. See details on page 8.

From Nov 1-7, I traveled to Japan to serve on the COE-21 Advisory Committee at the Institute for the Study of the Earth's Interior of Okayama University in Misasa. I also visited Spring-8, the Super Photon Ring, in Harima Science City, as a guest of Ken-ichi Funakoshi; while there, I gave a seminar on "Sound Velocities of Minerals under Mantle Conditions."

Recent issues of the newsletter of the National Synchrotron Light Source at the Brookhaven National Laboratory have highlighted achievements of members of the COMPRES community from Stony Brook University.

NSLS user Li Li is the 2006 recipient of the Alvin Van Valkenburg award. This international award is given every second year in the name of physicist Alvin Van Valkenburg, co-inventor of the diamond anvil cell, to honor a young scientist whose research The Van Valkenburg award was presented at the 2006 High Pressure Gordon Conference in Biddeford, Maine on June 29, 2006.

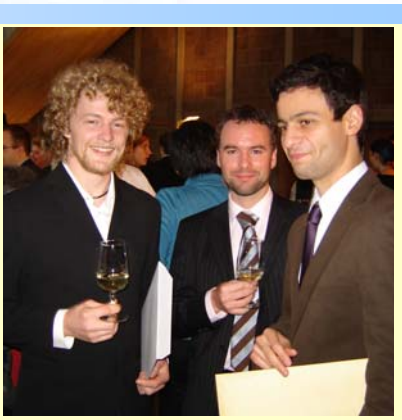
The Nov 8 science highlights from the NSLS featured a report on the work of Jiuhua Chen, Li Li, Tony Yu, Hongbo Long, Donald Weidner, Liping Wang and Michael Vaughan on "Breaking the Bounds of Plasticity" based on an article in the June 28, 2006 issue of the Journal of Physics: Condensed Matter.

On November 30, The Program Directors from the Division of Earth Sciences led a Site Visit from Instrumentation and Facilities Panel to the NSLS at Brookhaven, as part of the review of the proposal from COMPRES for renewed funding in the period 2007-2012. Nineteen members of our community represented COMPRES at the Site Visit. The oral presentations included introductory remarks by Bob Liebermann, a talk on the partnership of COMPRES and the NSLS by Chi-chang Kao [Director of NSLS and a member of the Advisory Committee of COMPRES], an overview of the program plans for COMPRES by Harry Green, and talks by representatives of the major users of COMPRES facilities [David Walker], leaders of infrastructure develop ment projects [both current and future], Kurt

(*continued on page 6*)

Artem R. Oganov (ETH Zurich) received the Latsis Prize (CHF 25,000) "for significant contributions to mineral physics, in particular for his works on crystal structure prediction and discovery of several major Earth-forming minerals" (November 8, 2006).

Colin W. Glass (ETH Zurich) received the ETH Zurich medal for an outstanding diploma work "USPEX - Evolutionary Crystal Structure Prediction" (November 18, 2006).



President's message (*cont'd*)

Leinenweber and Ho-kwang Mao. The Panel and the Program Directors of EAR also toured the beamlines at the NSLS operated with support from COMPRES led by Russell Hemley, Jiuhua Chen and Don Weidner, as well as a "virtual tour" of the high-pressure facilities at the ALS led by Simon Clark.

2007 Annual Meeting of COMPRES—Site and Dates now set.

Following a search by Ann Lattimore of potential sites for the 2007 Annual Meeting of COMPRES, the Executive Committee has settled on Lake Morey Resort in Fairlee, Vermont from Sunday, June 17 to Wednesday, June 20, 2007. See details of this site at: http://www.lakemoreyresort.com/TheResort.html

These dates were deliberately selected so that our Annual Meeting would follow immediately after the Gordon Research Conference on Earth's Interior, which will be held from June 10-15, 2007 at Mt Holyoke College in Massachusetts. We also wanted to find a site in the northeastern U. S. to optimize the proximity to Mt. Holyoke College.

Congratulations to Hans-Rudolf [Rudi] Wenk and his colleagues for organizing the very successful "MSA Workshop on Neutron Scattering in the Earth Sciences," which was held in Emeryville, California from Dec 7-9, 2006. COMPRES provided travel support for graduate student attendees to this Workshop. See also page 11.

Fall 2006 AGU Meeting in San Francisco.
This annual meeting included many highlights associated with the COMPRES community, including:

Excellent program of oral talks and poster presentations organized by Jennifer Jackson, formerly of the Carnegie Institution of Washington and as of December, an Assistant Professor at the California Institute of Technology in Pasadena.

Reception hosted by the Mineral and Rock Physics Focus Group
At this reception, the 2006 Outstanding Student Awards were presented to
Wendy Mao of the University of Chicago [Advisor: Dion Heinz].
Jungfeng Zhang of the University of California at Riverside [Advisor: Harry Green].

Exhibition booth jointly sponsored by GSECARS and COMPRES, which attracted lots of visitors. Our thanks to Jiuhua Chen for creating the PowerPoint presentation, to Ann Lattimore for overseeing preparations, and to Glenn Richard and Michael Vaughan for staffing the booth, as well as to Nancy Lazarz and Mark Rivers of GSECARS for their collaboration.

The Physical Properties of Earth Materials group once again organized a fantastic dinner celebration at the Citizen Thai and The Monkey Restaurant on the corner of Grant and Vallejo. Our congratulations to Brian Bonner and Steve Blair for discovering such a wonderful venue for this special evening.

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 14 to discuss the recommendations of the Standing Committees.

2006 MRP Outstanding Student Awardees:

Wendy Mao (PhD, Univ. Chicago, Aug. 2005) recognized for her doctoral research on the geophysics and geochemistry of iron in the Earth's core, and structure and elasticity of post-perovskite at deep mantle conditions.

Junfeng Zhang (PhD, Univ. California, Riverside, Oct. 2005) recognized for his doctoral research, the first experimental investigations of eclogite rheology, effects of hydrogen, and development of lattice preferred orientations during deformation (See *COMPRES Newsletter Vol.* 5 *No.* 1 for his dissertation abstract).

Alex Navrotsky awarded Harry H Hess Medal

Bob Liebermann, Alex Navrotsky and Charlie Prewitt at the award ceremony.

Charlie Prewitt and Bob Liebermann nominated Alex Navrotsky for AGU's 2006 Harry H. Hess Medal that was awarded in the Honors Ceremony at the Fall AGU Meeting. Bob and Charlie have known Alex for many years through contacts at meetings, conferences, and committees, and as a coauthor and colleague. Her efforts at Arizona State and Princeton were instrumental in opening up the field of mineral physics, and she helped to spearhead the effort that eventually led to the creation of CHiPR, the NSF Science and Technology Center, where for 11 years she served not only as a co-principal investigator but also was one of its most effective spokespersons. During this time, she was elected to the National Academy of Sciences and was the first woman faculty member to be so elected from Princeton University. As an example of her influence, Alex was the organizer of three extremely important conferences that have had a profound impact on subsequent activities in the mineral and materials sciences. One was the 1981 Castle Hot Springs conference in Wickenburg, Arizona, that brought together geoscientists, materials scientists, physicists, and chemists (including Linus Pauling) to discuss areas of common interest. Next was the Chapman Conference on "Perovskite - A Structure of Great Interest to Geophysics and Materials Science" held in Bisbee, Arizona, in 1987 and resulting in an AGU Monograph having the same title. The third was an NSF-sponsored workshop "Mineral and Rock Physics" held in Scottsdale, AZ, in 1999 which laid out directions for research in this area for the coming decade.

Alex has maintained a rather large research group of students, postdocs, and visitors throughout her academic career, and the productivity of this group is very high, thus attesting to her capacity for developing young scholars. From her many invitations from abroad to lecture or to take part in a variety of scientific activities, it is evident that her scientific reputation in international circles is as great as it is in the USA. COMPRES is fortunate to have Alex as an active and contributing member.

AWARD

COMPRES 6th Annual Meeting - Site and Dates

Lake Morey Resort in Fairlee, Vermont from Sunday, June 17 to Wednesday, June 20, 2007
Visit www.compres.us for meeting information update, www.lakemoreyresort.com/TheResort.html for conference site information.

COMPRES ANNUAL MEETING

A Symposium in Honor of Brian Evans

A portion of the Physical Properties of Earth Materials (PPEM) community gathered at MIT on 20-21 October 2006 to toast and roast one of PPEM's founding members, Brian Evans, on his 60th birthday. The symposium brought together many colleagues in the "friends of rock squeezers" community for three, one-half day sessions on themes loosely based on Brian's research interests over the last 30+ years:

Earth Materials - Deformation and Transport Properties
Massachusetts Institute of Technology, 20-21 October 2006

Brian the preacher

Yves Caristan, Peter Molnar Joe Walsh at the symposium

Brian the teacher

The presentations at the symposium were of very high quality, highlighting primarily new work by the authors with frequent references to Brian's contributions. The organizers are in discussions with the authors about documenting the presentations in a commemorative volume. For more information about the presentations contact the authors directly.

It's encouraging to see that fundamental science on the physical behavior of the Earth is alive and well, and that the rock squeezing community attracts interest from the peripheral disciplines of structural geology, seismology, geodynamics and materials sciences. I'm also pleased to see the growing crossover between academia and industry. Times have changed: I was pleasantly surprised to hear that many attendees - even from more academic research institutions -- are enthusiastically applying their current research to industry problems. With this growing emphasis on the potential applications of basic research, I encourage more members of PPEM to apply their expertise to the fascinating problems in industry.

The organizers of the symposium were Georg Dresen (GeoForschungsZentrum-Potsdam), Joanne Fredrich (BP) and Dave Olgaard (ExxonMobil). But the most difficult duties were assigned to David Kohlstedt and Steve Hickman who were responsible for finding humor in Brian's character to present at the evening reception and dinner. David took the easy approach by telling lies about Brian's early days at U. Minnesota etc., leaving honest Steve the difficult task of gathering silly antidotes from former students, post-docs and visitors of MIT and Princeton. Steve's job turned out to be

(*continued on page 9*)

SYMPOSIUM

Symposium, Brian Evans (*cont'd*)

Joe Walsh, Joanne Fredrich, Bill Brace and Brian disagreeing

quite a challenge! Although it won't end up on Jay Leno (Brian is no Steve Mackwell), because everyone was primed with dinner and significant quantities of libations, Steve was able to coax some hearty laughs and applause. I now have a third rule to add to my list for giving a successful talk: 1) State the obvious clearly (Brian Wernicke), 2) Take your change out of your pocket (Lisa Dell'Angelo), and 3) Don't [bleep] up (sage advice from Herr Professor Doctor Evans to a nervous graduate student giving his first AGU talk).

As many of you know, PPEM was the idea of Brian, Steve Kirby, Jan Tullis and Dave Kohlstedt; conceived, no doubt, after several ales and/or Chardonnays at the Edinburgh Castle, during a Fall AGU meeting. PPEM has survived nearly two decades on two basic principles: 1) the steering committee will primarily be made up of senior PPEM members who may not attend, and junior members who need justification to attend the Fall Meeting in San Francisco a few days early, and 2) to throw a dinner party at said meeting that is the envy of every other AGU subgroup. With these two principles, several dedicated volunteers, informative newsletters and e-mail communications, the annual dinner, and an active website, PPEM is thriving.

Lastly, the celebration would not have been a success without some key local support. First and foremost the organizing committee would like to thank Roberta Allard for her enthusiastic administrative help, the Department of Earth, Atmospheric and Planetary Sciences and MIT for providing the facilities, the MIT Media Center for ensuring that the audio and visuals worked without a hitch, the staff at GFZ-Potsdam for there pre and post-symposium time and help, and Bill Durham (who recently stepped down as the AGU party-man) as the *de facto* organizer on site. Finally, these projects require considerable financial help as well and for that we'd like to thank Statoil, Shell, BP and ExxonMobil.

Happy Birthday Brian! Good times were had by all… Now, who's over-the-hill next?

— Dave Olgaard
Photographed and captioned by David Kohlstedt

Exhibition booth jointly sponsored by COMPRES and GSECARS at Fall 2006 AGU Meeting

The exhibition booth staffed by Glenn Richard and Michael Vaughan from Stony Brook University and Nancy Lazarz and Mark Rivers from GSECARS attracted a number of visitor. Both COMPRES and GSECARS supplied handouts for information about their facilities. Photo on the left: Glenn Richard at the booth.

Recent PhDs

Kimberly Tait
Ph.D. 2007

University of Arizona

Dissertation: **X-ray and neutron studies of gas hydrates and sulfides at various pressures and temperatures**

Part I:

Gas hydrates (clathrates) are elevated-pressure (*P*) and low-temperature (*T*) solid phases in which gas molecule guests are physically incorporated into hydrogen-bonded, cage-like ice host frameworks.

Storage of hydrogen in molecular form within a clathrate framework has been one of the suggested methods for storing hydrogen fuel safely, but pure hydrogen clathrates form at high pressures (~2 kbar), which makes them impractical as a solution for hydrogen storage. Recent work has demonstrated that it is possible to obtain up to 4 wt% hydrogen in ice clathrates when tetrahydrofuran (THF) is used to promote the formation of the clathrates structure and hydrogen takes up double occupancy of the small cage and then also starts to fill the larger cages as the THF concentration is reduced. Neutron INS measurements on hydrogen adsorbed in d-THF+H_2/D_2O ice clathrate were carried out on the Pharos spectrometer at LANSCE. Experiments at 8K yielded two excitations at neutron energy gains of approximately 14 and 4.7 meV as compared with the H_2 free rotor separation of 14.7 meV. These can only arise from two species of hydrogen adsorbed in the clathrate, under the influence of quite different crystal fields. We also have been looking at other hydrogen-storage materials using Pharos and FDS, the two inelastic neutron scattering instruments at LANSCE.

Part II:

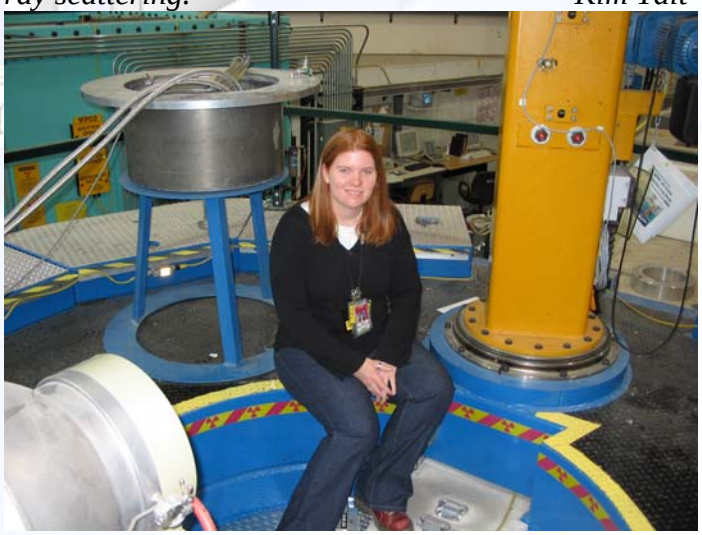
Metal sulfides are a geological ubiquitous group of minerals that display a host of interesting bonding interactions and structure types as well as an assortment of important electronic and magnetic properties. A great deal of work has been done with metal oxides that display a more simple bonding structure, but to date very little work has been done on describing the more complex metal-metal, sulfur-sulfur and metal-sulfur bonding in the sulfides.

We have synthesized a suite of highly crystalline, transition-metal sulfides of varying compositions and have studied several samples at high *P* (and *T*, where possible) to further the understanding of these complicated materials.

Statement:

I have had a great experience as a graduate student- my graduate student advisor was Dr. Robert Downs in the Geosciences Department at the University of Arizona. Although I spent most of my time at Los Alamos, Bob was always supportive via email and always at the other end of my phone call if I had any questions or just needed advice. I was introduced to the world of neutron scattering at the Los Alamos Neutron Scattering Center (LANSCE) where Dr. Yusheng Zhao was my mentor, and worked closely and learned a great deal from Luke Daemen, Frans Trouw, Darrick Williams and Monika Hartl at LANSCE. I would also like to thank Charlie Prewitt, now at the University of Arizona, for his invaluable input and insight on my thesis committee.

I was very fortunate to travel to several synchrotron and neutron sources across the United States and thank (especially) the staff at HPCAT at the APS for being so helpful for my many visits there. I look forward to my new position at the Royal Ontario Museum in Toronto, Ontario Canada as Associate Curator of Mineralogy starting April 2, 2007 where I plan on continuing work on high pressure neutron and X-ray scattering. — *Kim Tait*



Kim Tait at NPDF (the Neutron Powder Diffractometer) of the Los Alamos National Laboratory. She will defend her thesis in March.

COMPRES Sponsored Workshop

MSA Short Course on Neutron Scattering in Earth Sciences

A Short Course on Neutron Scattering in Earth Sciences was convened by Rudy Wenk (UC Berkeley) and Nancy Ross (VPI) December 7th and 8th, 2006 in Emeryville, California. It attracted 65 participants, including 16 students. Generous support from DOE-BES as well as COMPRES made it possible to keep registration costs at a minimum, particularly for students. Lectures given by a group of international experts covered a wide range of topics, from elastic scattering and diffraction to inelastic scattering and analysis of the structure of liquids. Possibilities for high pressure experiments at the future SNAP beamline of SNS raised a lot of interest. A volume covering the various topics (#63 in the Series of Reviews in Mineralogy and Geochemistry) was distributed at the meeting and will no doubt become a useful introduction to neutron scattering. The response from participants was enthusiastic and hopefully will stimulate new earth science neutron users. The Short Course was followed by a 1-day Workshop in Berkeley with 45 attending. It was dedicated to data analysis from TOF neutron diffractometers such as HIPPO at LANSCE and finished with hands-on Rietveld analysis, simultaneously with two codes, GSAS and MAUD. They finished at about the same time and very similar results. This was a good reason to celebrate with a final reception before adjourning.

In the photo (by Wenqian Xu): From left to right: S. Choi, W. Kuhs, R. Von Dreele, L. Lutterotti, J. Gomez Barreiro, R. Wenk, C. Jones, M. Voltolini, S. Fukura, S. Agnew, B. Chen, S. Vogel

COMPRES Sponsored Workshop

COMPRES upcoming workshop

Current vision and prospects for establishing of the high-pressure scale at high temperature

Jan 26-28, Washington D.C., Geophysical Laboratory

Organized by Alexander Goncharov, Kurt Leinenweber, Tom Duffy, Russell Hemley, Yingwei Fei

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