

COMPRES Annual Report

Nov. 1, 2015 - Oct. 30, 2016

Wenli Bi

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I have been working at sector 3, APS since Nov. 2011, first as a joint Postdoctoral Research Associate with COMPRES (Nov.2011- Jan. 2015), and recently as a Visiting Spectroscopist since Feb. 2015, supervised by Prof. Jay Bass (UIUC) and Dr. Ercan Alp (ANL). My responsibilities include assisting users with experiments involving Nuclear Resonant and Momentum Resolved Inelastic X-ray Scattering at sector 3 (NRS and IXS), the development of instrumentation and techniques for high-pressure Earth Sciences applications of IXS and Mössbauer spectroscopy, being the interface between potential users in the COMPRES community and the beamlines, working with members of the COMPRES community to develop competitive proposals for beamtime, and organizing workshops on NRS and IXS techniques.

This position is 70% supported by COMRPES and 30% supported by the APS. I have been spending about 70% of my time on COMPRES-related activities and 30% on other research activities.

Activities

During the past year I have been working at the sector 3 beamlines as well as the offline conventional Mössbauer Lab, assisting users primarily from the COMPRES community to carry out experiments, characterizing samples, and conducting my own research.

I have helped users with beamtime proposal writing, beamline experimental setup, diamond anvil cell preparation, sample loading, data collection, and analysis. I also have helped users at sector 3 to install CONUSS and PHOENIX softwares on their computers and trained new users on how to analyze data. For experiments at the Mössbauer lab I have helped run measurements and analyzed data of various samples from users at ambient conditions as well as at high pressure or low temperature conditions. In a majority of cases, I do all or nearly all of the data collection and analysis for Mössbauer experiments.

I have lead the development of the new capability of high pressure and low temperature (HPLT) nuclear resonant inelastic x-ray scattering (NRIXS) at sector 3, a 2-year PUP with COMPRES. We have developed a miniature panoramic DAC, a cryostat with liquid helium flow further down to the DAC holder, and an efficient gas-membrane driven system to tune pressure in-situ. This instrumentation is a technical breakthrough to enable NRIXS experiment at HP-LT conditions.

We recently acquired the offline Raman system previously located at GSECARS. I have been maintaining the system and trained new users in how to operate and take data. I maintain the glovebox at sector 3, help users with sample loadings from sector 3 and also sector 30, and gas loading at GSECARS in panoramic DACs.

List of scientific projects involved:

1. At sector 3, sector 30 and HPCAT
 - (1) Development of High-Pressure and Low-Temperature Nuclear Resonant Scattering Capability for Geoscience and Condensed Matter Physics Applications at 3-ID (PUP). The PUP was allocated 6 days of beamtime in each cycle for two years of period (2014-2016). Lead the project, commissioned the recently developed setup for high pressure and low temperature NRIXS experiments.
 - (2) Exploitation of the hybrid-filling mode of the APS to map out the pressure-temperature phase diagram of iron metal (self-PI). This project is aimed to explore the hybrid mode for applications in mineral physics. The extended time window of 1 micro-second in this timing mode allows more accurate determination of valence, spin and magnetic state.
 - (3) Pressure-induced magnetic transitions in greigite (Fe_3S_4). Collaboration with John Tse from University of Saskatchewan. Prepared DAC, loaded sample, focused x-ray, took beamtime, collected and analyzed data.
 - (4) Mössbauer microscopic investigation of disproportionation of ferrous ions into metallic iron and ferric ions under pressure. Collaboration with Prof. Shun-ichiro Karato's group. Helped with beamline setup, helped with data evaluation and trained postdoc with data analysis.
 - (5) The high-pressure phonon density of states of fcc iron hydride (Andrew Campbell, U. of Chicago). Trained student with DAC and Be gasket preparation. Helped with beamline setup, data collection and data evaluation.
 - (6) Studies of isotope fractionation in basalts under pressure (Jung-fu Lin, UTexas Austin). Helped with beamline setup, x-ray focusing, data evaluation. Taught student beamline operation and data analysis.
 - (7) Studies of magnetism in Dy by synchrotron Mössbauer spectroscopy at Extreme Pressures (self-PI). A manuscript is in preparation.
 - (8) The role of phonon softening in the pressure-induced amorphization process of the tin-halide molecular crystals SnBr_4 and $\text{Sn}(\text{BrI})_2$ (PI: Michael Hu, APS). Prepared DAC, loaded sample, carried out experiment at sector 30.
 - (9) Characterizing MgFeSiO_3 samples under pressure to determine the spin state in perovskite and post-perovskite phases (Thomas Duffy's group). Took beamtime, collected and analyzed data.
 - (10) Presence of ferric iron in single crystal magnesiowuestite (Jennifer Jackson, Caltech). Helped with experiment setup.
 - (11) Magnetic phase diagram of iron hydride under extreme pressures (Viktor Struzhkin, CIW). Helped the user to prepare mini-panoramic DACs, worked

on beamline setup including x-ray focusing, cell/membrane assembly, cryostat and online Raman system (loan from HPCAT). Taught user with beamline operation and data analysis.

- (12) Spin and valence state of FeO_2 and FeO_2H_x (Jin Liu, Wendy Mao's group, Stanford U). Helped with experiment at HPCAT and analyzed data. Taught user about data analysis.
- (13) Studies of pressure-induced phonon anomaly in Sb (Raphael Hermann, ORNL). Prepared DAC, loaded samples and applied pressures during HERIXS beamtime at sector 30.
- (14) Pressure-induced phonon behaviors of TiO_2 (John Budai, ORNL). Prepared DAC loaded samples for HERIXS beamtime at sector 30.

2. In the offline Mössbauer lab, we have two independently running Mössbauer spectrometers. I run samples to support beamline projects, as well as independent experiments as requested by researchers across the country. In the period of past year over 30 samples from 10 groups have been measured in the lab.

Beamtime Proposals I have involved in writing:

- (1) Spin state of transitions of Fe in $(\text{Mg,Fe})\text{GeO}_3$ using synchrotron Mössbauer spectroscopy (GUP-46440, Tom Duffy's group from Princeton University)
- (2) The high pressure phonon density of states of fcc iron hydride (GUP-40453, Andrew Campbell's group from University of Chicago)
- (3) Mössbauer microscopic investigation of disproportionation of ferrous ions into metallic iron and ferric ions under pressure (GUP-43134, Shun-ichiro Karato's group, Yale University)
- (4) Synchrotron Mössbauer Spectroscopy (SMS) Studies of the Magnetic State in Dy under Extreme Pressure (GUP-40395, self-PI)
- (5) Lattice dynamice study of pressure-induced amorphization in the SnBr_2I_2 molecular crystals (GUP-40200, Michael Hu, ANL)

Education, Outreach, Workshop and Community service:

- (1) Organizing and chairing the upcoming Workshop on Nuclear Resonant Scattering and Data Analysis on Nov. 11-13, 2016 at the APS, ANL.
- (2) Helped user groups with general user proposal writing for beamtime, trained new users with data acquisition and data analysis, helped new users to install CONUSS and PHOENIX packages for data analysis.
- (3) Run the offline Mössbauer lab. Collect spectra, analyze, and interpret data for COMPRES users.
- (4) Actively participated the 2016 COMPRES meeting. Presented a poster titled "Studies of the α - ϵ Transformation in Iron at Various Temperatures by Synchrotron Mössbauer Spectroscopy (SMS) in Hybrid Mode".
- (5) Lead and completed the PUP-38969 titled Development of High-Pressure and Low-Temperature Nuclear Resonant Scattering Capability for Geoscience and Condensed Matter Physics Applications at 3-ID.

Invited and Contributed presentations

Nature of phase transitions in EuFe_2As_2 studied by ^{57}Fe and ^{151}Eu Nuclear Resonant Scattering (NRS) under high pressure, poster at High Pressure, Research at Gordon Research Conference, Holderness, NH, July 2016.

Studies of the α - ϵ Transformation in Iron at Various Temperatures by Synchrotron Mössbauer Spectroscopy (SMS) in Hybrid Mode, poster presentation at 2016 COMPRES annual meeting. NM, June, 2016.

Studies of pressure effect on magnetism via synchrotron Mössbauer spectroscopy, talk at APS User Science seminar, April 2016.

Probing Magnetism and Lattice Dynamics via Nuclear Resonant Scattering, invited talk at the Condensed Matter Physics Seminar, Washington University in St. Louis, March 2016.

List of recent publications

Mathieu Roskosz, Corliss K.I. Sio, Nicolas Dauphas, **Wenli Bi**, François L.H. Tissot, Michael Y. Hu, Jiyong Zhao, Esen E. Alp, *Spinel–olivine–pyroxene equilibrium iron isotopic fractionation and applications to natural peridotites*, *Geochim. Cosmochim. Acta* **169**, 184-199 (2015).

Jamie Y. C. Chen, Lianna Dang, Hanfeng Liang, **Wenli Bi**, James B. Gerken, Song Jin, E. Ercan Alp, Shannon S. Stahl, *Operando Analysis of NiFe- and Fe-Oxide Electrocatalysts for Water Oxidation: Detection of Fe^{+4} by Mössbauer Spectroscopy*,¹ *J. Am. Chem. Soc.* **137**, 15090 (2015).

H. Liu, J.S. Tse, M.Y. Hu, **W. Bi**, J. Zhao, E.E. Alp, M. Pasternak, R.D. Taylor, and J.C. Lashley, *Mechanisms for pressure-induced crystal-crystal transition, amorphization, and devitrification of SnI_4* , *J. Chem. Phys.* **143**, 164508 (2015).

Y. Choi, X. Jiang, **W. Bi**, P. Lapa, R. K. Chouhan, D. Paudyal, T. Varga, D. Popov, J. Cui, D. Haskel, J. S. Jiang, *Element resolved magnetism across the temperature- and pressure-induced spin reorientation in MnBi* , *Phys. Rev. B.*, accepted for publication.

W. Bi, J. Lim, G. Fabbri, J. Zhao, D. Haskel, E.E. Alp, M.Y. Hu, P. Chow, Y. Xiao, W. Xu, and J.S. Schilling, *Magnetism of europium under extreme pressures*, *Phys. Rev. B* **93**, 184424 (2016).

Y.Q. Wang, P.C. Lu, J.J. Wu, J. Liu, X.C. Wang, J.Y. Zhao, W. Bi, E.E. Alp, C.Y. Park, D. Popov, C.Q. Jin, J. Sun, and J.F. Lin, *Phonon density of states of single-crystal SrFe_2As_2 across the collapsed phase transition at high pressure*, *Phys. Rev. B.* **94**, 014516 (2016).

C. Li, Z. Yu, W. Bi, J. Zhao, M.Y. Hu, J. Zhao, W. Wu, J. Luo, H. Yan, E.E. Alp, and H. Liu, *In situ high-pressure synchrotron Mössbauer and X-ray diffraction studies: exploring the structure-related valence fluctuating in EuNi_2P_2* , Phys. B Condens. Matter **501**, 101 (2016).

Jin Liu, Nicolas Dauphas, Jung-Fu Lin, Mathieu Roskosz, Michael Y. Hu, Hong Yang, **Wenli Bi**, Jiyong Zhao, *Iron isotopic fractionation between silicate mantle and metallic iron core under high-pressure core formation conditions*, under review.