

COMPRES Annual Report

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Basic information

I have been working at sector 3, APS, ANL since Nov., 2011, first as a joint Postdoctoral Research Associate with COMPRES (Nov. 2011- Jan. 2015), then as a Visiting Spectroscopist from Feb. 2015 to May 2017, and then as a Senior Spectroscopist since June 2017, under the supervision of Prof. Jay Bass (UIUC) and Dr. Ercan Alp (APS, ANL).

My responsibilities include assisting users with experiments involving Nuclear Resonant and Momentum Resolved Inelastic X-ray Scattering at sector 3 and 30 (NRS and IXS), development of instrumentation and techniques for high-pressure Earth Sciences applications of IXS and Mössbauer spectroscopy, being the interface between 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 supported approximately 60% by COMRPES and 40% by the APS, ANL.

Activities

During the period of this report I have been working at the sector 3 and 30 beamlines as well as the offline conventional Mössbauer Lab, primarily assisting users from COMPRES, with some involvement in projects of non-COMPRES users for personal enrichment and advancement, carrying out experiments, characterizing samples, organizing NRS workshops, and conducting my own research to pursue my personal research interests and advance my scientific career.

I have been involving with beamtime proposal writing, beamline experimental setup, diamond anvil cell preparation, sample loading, data collection, and online/offline data analysis. I also have trained new users on how to analyze data and helped NRS users to install CONUSS and PHOENIX software on their computers. For experiments at the conventional Mössbauer lab I have performed experiments and data analysis for mail-in and drop-off samples from users at ambient as well as high pressure conditions.

I have been maintaining the offline Raman system at Sector 3 lab and training new users with system operation and data collection. The offline Raman system has been used routinely by users from Sector 3 and other beamlines. During the last year 15 research groups have used the system over 40 times for pressure measurements from either ruby fluorescence and/or diamond Raman edge.

I have maintained the glovebox and high-pressure instruments at sector 3, supported high-pressure users at Sector 3, Sector 30 and Sector 27, including DAC preparation, sample loading, and carrying out high-pressure experiments.

Scientific projects involved

The specific tasks I perform with users varies greatly, depending on the experience of users and the nature of the projects. My contributions include beamtime proposal writing, training users in the use of diamond cells and other high pressure equipment, loading samples and inert gas pressure media, instruction on how to operate the beamline and collect data, data collection, data analysis using the CONUSS and PHOENIX software packages, instruction on data analysis, pressure measurement, and helping to write manuscripts. Again, the amount of direct participation, for example sample prep, data collection, analysis, and instruction on all the above, varies widely from user to user. There is typically student/postdoc turnover and new student users each year, who need a high level of support to begin experiments. All experiments involved a certain amount of beamline setup prior to the experiments, which cannot be done by even experienced users.

A list of projects I directly participated in at Sector 3, 30 and other beamlines are as follows.

1. Iron bonding environment and its isotope fractionation factors in silicate glasses at high pressures: SMS and NRIXS studies in a diamond anvil cell (GUP-51818, Jung-Fu Lin's group, UT-Austin).
2. Phonon density of states and sound velocities in the lower mantle (GUP-50312, Wendy Mao's group, Stanford U.).
3. Valence electron states of iron in Ca-bearing bridgmanite (GUP-52033, Dan Shim's group, ASU).
4. Acoustic properties of Fe_3P up to core pressures by nuclear resonant inelastic x-ray scattering (GUP-57700, Bin Chen, U. of Hawaii).
5. Determining Fe isotopic fractionation factors between natural minerals using NRIXS (GUP-59387, Nicolas Dauphas, U. of Chicago).
6. Studies of magnetic transitions of jarosite under pressure (Danna Freedman's group, Northwestern U.).
7. Studies of isomer shift of Fe under pressure up to 1 Mbar using synchrotron Mössbauer spectroscopy (collaboration with John Tse, U. of Saskatchewan).
8. The effect of tin coordination number on the tin isotope fractionation factors in high-pressure polymorphs of SnO_2 (GUP-53262, Mathieu Roskosz, Muséum National d'Histoire Naturelle).
9. Melting investigations of Fe-Ni-Si at high-pressure using synchrotron Mössbauer spectroscopy and fast temperature detection (GUP-58399, Jennifer Jackson's group, Caltech).
10. NRIXS study in equilibrium fractionation of europium and dysprosium in minerals and synthesized glass: defining the baseline of REE isotopic fractionation in nature (GUP-58739, N. Dauphas, U. of Chicago).
11. Sound velocities and spin state of Fe-bearing delta- AlOOH : Implications for the deep water cycle (GUP-51689, Jennifer Jackson, Caltech).
12. Studies of magnetism in KBiFe_2O_5 under pressure: a new type of oxygen-deficient, ordered double perovskite (collaboration with Yonggang Wang, HPSTAR).
13. Nematic fluctuations in superconducting FeSe under pressure (GUP-54808, Dmitry Reznik, U. of Colorado Boulder).

14. Sn-partial phonon DOS across pressure-induced phase transition in anharmonic SnSe (GUP-52093, Oliver Delaire, Duke U.).
15. Investigation of phonon modes of CaLa_2 at pressure-induced bi-critical point using Inelastic X-ray Scattering (GUP-56992, Sara Haravifard's group, Duke U.)
16. High pressure studies of magnetism and valence in novel $\text{EuAFe}_4\text{As}_4$ ($A=\text{Cs, Rb}$) superconductors using synchrotron Mössbauer spectroscopy (GUP-53898, self-PI).
17. ^{151}Eu synchrotron Mössbauer spectroscopy study of the temperature and pressure dependence of intermediate valence and magnetic ordering in $\text{Ca}_{1-x}\text{Eu}_x\text{Co}_2\text{As}_2$ (GUP-54626, Michael Shatruk, FSU).
18. Studies of magnetism in FeP under pressure (Philipp Materne, APS)
19. Mapping of iron speciations and phase transformations in ultrahard Chiton teeth using cryogenic Mössbauer microscopy (GUP-55167, Linus Stebauer, Northwestern U.)
20. Synchrotron Mössbauer exploration of antiferromagnetic order in EuGa_4 and EuAl_4 under pressure and the fate of local moments (GUP-60770, Yejun Feng, OIST)
21. Studies of phonon dispersion and electronic transitions of GaTa_4Se_8 under pressure using RIXS and HERIXS at Sector 27 and Sector 30 (GUP-55877, Jungho Kim, APS).
22. Mentored Dr. Philipp Materne (Jan. 2017-Dec. 2018), a postdoc at Sector 3, on high pressure experiments and beamline operation, data analysis, etc. Collaborated with Dr. Materne on various projects of magnetic studies of various Fe-containing systems at high pressure and low temperature conditions (GUP-53291, 57027, 58657).
23. XANES studies of the valence state of Yb under extreme pressure (collaboration with James Schilling's group, WashU).

Other than the activities at beamlines, I also provide services in the offline conventional Mössbauer lab, taking data on mail-in or drop-off samples from users. My activities in the offline Mössbauer lab included prepare ambient samples, taking Mössbauer data, changing pressure in DACs for high pressure experiments, and analyzing data for users. During the last year, over 30 samples from 13 COMPRES groups have been measured at ambient as well as high pressure conditions.

Education and Outreach

- Organized the NRS Workshop 2018: Nuclear Resonant Inelastic X-ray Scattering and Data Analysis, Nov. 2-4, 2018 at the Advanced Photon Source, Argonne National Laboratory.
- Active participation in the COMPRES annual meeting with oral presentations and posters.
- Year-round training of users for beamline experiment operation and data analysis.
- Offered mail-in service to COMPRES users at the Mössbauer lab.

Invited and Contributed presentations

- *Nuclear resonant scattering studies of magnetism and valence in Eu- and Dy-based systems: pnictides and SMMs*, invited talk at the Workshop on Discovery, Synthesis, and Development of Emerging Materials and the Role of the APS Upgrade, Sept., 2018, APS, ANL.
- *Workshop on CONUSS and Synchrotron Mössbauer Data Analysis*, report at the COMPRES annual meeting, August, 2018, NM.
- *Inelastic and Nuclear Resonant X-ray Scattering at the Advanced Photon Source (Sectors 3ID and 30ID)*, poster presentation at the COMPRES annual meeting, August, 2018, NM.

- *Application of Synchrotron Mössbauer Spectroscopy (^{57}Fe , ^{151}Eu , ^{161}Dy) in studies of magnetism under high pressure*, poster presentation at the GRC-Research at High Pressure, July, 2018, NH.
- *Studies of magnetism in dysprosium under extreme pressures*, poster presentation at the APS Users Meeting, May, 2018, APS, ANL.
- *High pressure studies of magnetism via synchrotron Mössbauer spectroscopy at Symposium on matter at high and ultra-high pressures*, April 2018, St. Louis, MO.

List of publications since Nov. 2017

1. Chen B., Lai X., Li J., Liu, J., Zhao J., **Bi W.**, Alp E. E., Hu M. Y. & Xiao Y., Experimental constraints on the sound velocities of cementite Fe_3C to core pressures, *Earth Planet. Sci. Lett.* **494**, 164-171, 2018.
2. Klein R. A., Walsh J. P. S., Clarke S. M., Guo Y., **Bi W.**, Fabbri G., Meng Y., Haskel D., Alp E. E., Duyn R. P. Van, Jacobsen S. D. & Freeman D. E., Impact of pressure on magnetic order in jarosite, *J. Am. Chem. Soc.* **140**, 12001, 2018.
3. Malavi P., Song J., **Bi W.**, Regnat A., Senyshyn A., Pflleiderer C. & Schilling J. S., High-pressure investigations on the semi-Heusler compound CuMnSb , *Phys. Rev. B.* **98**, 054431, 2018.
4. Jackson D. E., VanGennep D., **Bi W.**, Zhang D., Materne P., Liu, Y. Cao, G.-H., Weir S. T., Vohra Y. K. & Hamlin J. J., Superconducting and magnetic phase diagram of $\text{RbEuFe}_4\text{As}_4$ and $\text{CsEuFe}_4\text{As}_4$ at high pressure, *Phys. Rev. B.* **98**, 014518, 2018.
5. Song J., Fabbri G., Bi W., Haskel D. & Schilling J. S., Pressure-induced superconductivity in elemental ytterbium metal, *Phys. Rev. Lett.* **121**, 037004, 2018.
6. Materne P., **Bi W.**, Alp E.E., Zhao J., Hu M. Y., Jesche A., Geibel C., Kappenberger R., Aswartham S., Wurmehl S., Büchner B., Zhang D., Goltz T., Spehling J. & Klauss H. *Phys. Rev. B.* **98**, 14517, 2018.
7. Thompson E.C., Davis A. H., **Bi W.**, Zhao J., Alp E. E., Zhang D., Greenberg E., Prakapenka V. B. & Campbell A. J., High-pressure geophysical properties of fcc phase FeH_x , *Geochemistry, Geophys. Geosystems.* **19**, 305-314, 2018.
8. Fei Y., Iqbal M., Kong S. D., Xue Z., McFadden C. P., Guillet J. L., Doerrer L. H., Alp E. E., **Bi W.**, Lu Y., Dandamudi C. B., Ranganath P. J., Javier K. J., Ahmadian M., Ellison C. J. & Johnston K. P., Aqueous Superparamagnetic magnetite dispersions with ultrahigh initial magnetic susceptibilities, *Langmuir.* **34**, 622–629, 2018.
9. Liu J., Dorfman S. M., Zhu F., Li J., Wang Y., Zhang D., Xiao Y., **Bi W.** & Alp, E. E., Valence and spin states of iron are invisible in Earth's lower mantle, *Nat. Commun.* **9**, 1284, 2018.
10. Yang H., Lin J-F., Hu M.Y., Roskosz M., **Bi W.**, Zhao J., Alp E.E., Liu J., Liu J., Wentzowitch R.M., Okuchi T., Dauphas N., Iron isotopic fractionation in mineral phases from earth's lower mantle: did terrestrial magma ocean crystallization fractionate iron isotopes? *Earth Planet. Sci. Lett.* **506**, 113, 2019.
11. Materne P., **Bi W.**, Alp E.E., Zhao J., Hu M. Y., Jesche A., Geibel C., Kappenberger R., Aswartham S., Wurmehl S., Büchner B., Zhang D., Goltz T., Spehling J. & Klauss H., Bandwidth controlled insulator-metal transition in BaFe_2S_3 : a Mössbauer study under pressure, *Phys., Rev. B* (under review) 2018.
12. Materne P., **Bi W.**, Zhao J., Hu M.Y., Alp E. E., Kappenberger R., Aswartham S., Wurmehl S., Büchner B., Microscopic phase diagram of LaFeAsO single crystals under pressure, *Phys. Rev. B* (accepted) 2018.

13. Zhao J. Y., **Bi W.**, Sinogeikin S., Hu M.Y., Alp E. E., Lin J. F., Jin C. Q., A compact membrane-driven diamond anvil cell and cryostat system for nuclear resonant scattering at high pressure and low temperature, *Rev. Sci. Instrum.* **88**, 125109, 2017.
14. Dauphas N., Hu M.Y., Baker E.M., Hu J., Tissot F.L.H., Alp E.E., Roskosz M., Zhao J., **Bi W.**, Liu J., Lin J-F., Nie N.X., Heard A., SciPhon: a data analysis software for nuclear resonant inelastic X-ray scattering with applications to Fe, Kr, Sn, Eu, and Dy, *J. Synchrotron Rad.* **25**, 1581, 2018.
15. Materne P., **Bi W.**, Alp E. E., Zhao J., Hu M. Y., Jesche A., Geibel C., Kappenberger R., Aswartham S., Wurmehl S., Büchner B., Zhang D., Goltz T., Spehling J. & Klauss H. H., *Phys. Rev. B.* **98**, 14517, 2018.
16. Ying J., Zhao J., **Bi W.**, Alp E.E., Xiao Y., Chow P. and Struzhkin V.V., Unexpected complex magnetic phase diagram of ϵ' -FeH, (submitted) 2018.
17. Liu J., Wang W., Dauphas N., Yang H., Wu Z., Hu M.Y., Zhao J., **Bi W.**, Alp E.E., Liang W., Chen B., Lin J-F., Carbon isotopic signatures of diamond formation mediated by iron redox chemistry, *Geochem. Perp. Let.* (submitted) 2018.
18. Liu J., Hu Q., **Bi W.**, Yang L., Xiao Y., Chow P., Meng Y., Prakapenka V.B., Mao H-K., Mao W.L., Altered chemistry of O, Fe and H in the middle Earth, *Nat. Commun.* (under review) 2018.