

Annual Report of Year 2013-2014

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Since November 2011, I have been working at sector 3, APS as a joint Postdoctoral Research Associate with COMPRES. The duties of this position include (but not limited to) 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 Mossbauer 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

From October 2013, I have been working at the sector 3 beamlines and at the conventional Mössbauer spectroscopy Lab affiliated to the beamline, assisting users from both COMPRES and non-COMPRES community carrying out experiments, characterizing samples, and conducting my own research.

I have helped users with 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 their NRS data. For experiments at conventional 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.

I have been heavily involved in developing the new capability of high pressure and low temperature (HPLT) nuclear resonant inelastic x-ray scattering (NRIXS) at sector 3. I have tested the new cryostat, integrated the setup, and commissioned the new capability in the studies of spin, magnetism, valence and lattice dynamics in EuFe_2As_2 under high pressure and low temperature with both ^{57}Fe and ^{151}Eu isotopes. I have assisted general proposal users in the HPLT NRIXS experiments. Based on the problems I found during testing and commissioning runs, I suggested modifications for the next version cryostat and diamond anvil cell design. Currently we are designing a new cryostat to reach 4 Kelvin and a membrane system to be able to tune pressure in-situ.

I also helped Dr. Jiyong Zhao to maintain the glovebox at sector 3. I helped users with sample loadings inside the glovebox and gas loading at GSECARS in the panoramic DAC.

Here is a list of scientific projects I have involved:

1. At sector 3 and other beamlines

- (1) High Pressure Studies of Spin, Magnetism, Valence, and Lattice dynamics in EuFe_2As_2 using Nuclear Resonant Scattering (GUP-32955, self-PI). This is a project I am interested in independently, also in collaboration with Jung-Fu Lin.
- (2) Studies of 4f local moment in Eu by X-ray Emission Spectroscopy (XES) at Extreme Pressures (GUP-34050, self-PI). This is a project in collaboration with my Prof. James Schilling, Washington University in St. Louis.
- (3) Phonon density of states of ferropnictide superconductors at high pressures and low temperatures by nuclear resonant inelastic X-ray scattering (GUP-37536, Jung-Fu Lin's group). I set up the cryostat, helped in DAC preparation, sample loading and Ne pressure medium loading, x-ray monochromation and focusing, and data analysis.
- (4) Sound velocities of Fe_7C_3 up to 1 Mbar and 1800 K by nuclear resonant inelastic x-ray scattering (GUP-31100, PI: B. Chen). I helped with x-ray monochromation and focusing, and data reduction.
- (5) Effect of temperature on the sound velocities of Fe_7C_3 at pressures up to 150 GPa (GUP-39186, PI: B. Chen). I helped with laser heating optics alignment, x-ray monochromation and focusing, and data reduction. Trained the students how to analyzed data.
- (6) Nuclear Forward Scattering of Pyrolytic and Basaltic Mantle-Silicate Perovskites (GUP-37084, PI: Dan Shim). Helped with x-ray monochromation and focusing, and data reduction.
- (7) The role of phonon softening in the pressure-induced amorphization process of the tin-halide molecular crystals SnI_4 and SnBr_4 (in collaboration with M. Pasternak from Tel Aviv University and Dean Taylor from Los Alamos). I prepared the DAC, loaded sample and helped with x-ray monochromation and focusing, data collection and analysis.
- (8) Temperature and redox effects on the iron phonon density of states of silicate glasses and olivine (GUP-35993, PI: N. Dauphas, U of Chicago). Helped with x-ray monochromation and focusing, and data reduction.
- (9) Temperature effect on the elastic properties of single crystal bcc iron under pressure (GUP-37691, Jung-Fu Lin's group). Took beamtime and helped in data collection.
- (10) Characterization of recovered olivine sample after high temperature and high pressure experiment (with Jin Zhang from Jay Bass's group). Took beamtime and collected and analyzed data. Installed softwares in Jin's computer and

taught her how to analyze data.

- (11) Characterizing MgFeSiO₃ samples under pressure to determine the spin state of MgFeSiO₃ in perovskite and post-perovskite phases (Thomas Duffy's group). Took beamtime, collected and analyzed data.
- (12) Equilibrium iron isotope fractionation in the Earth's lower mantle (GUP-39191, Jung-Fu Lin's group). Helped with x-ray monochromation and focusing, and data reduction.
- (13) High Pressure Synchrotron Mössbauer Spectroscopy (SMS) on Mixed Valence Tri-nuclear Iron Complexes – Fe₃O(Carboxylate)₆(Ligand)₃ - and Photomagnetic Switchable Materials – MFeDMF (GUP-37591, B. Iversen, Aarhus University, Denmark), Helped with diamond anvil cell preparation, sample loading, gas loading as pressure medium, membrane DAC setup, x-ray monochromation and focusing, and data analysis.
- (14) Phonon density of states of hcp-Fe up to 360 GPa by NRIXS (GUP-30939, Jung-Fu Lin's group). Helped with x-ray monochromation and focusing, and data reduction.
- (15) Investigation of low temperature magnetic structure of superconducting FeTeO(x) films (GUP-37262, Barret Wells's group, University of Connecticut). Helped with cryostat setup, x-ray monochromation and focusing, and data analysis.
- (16) Origin of Jahn-Teller distortion and high-low spin transition of Fe₂TiO₄, and FeCr₂O₄ and their pressure-induced structure transformation (GUP-32556, Takamitsu Yamanaka, CIW). Helped with data analysis.

2. At Mössbauer lab, there are two independently running Mössbauer spectrometers. I run samples to support beamline projects, as well as independent experiments as requested by researchers around the country.

- (1) Characterization of spinel samples and rocks from New Zealand from N. Dauphas, University of Chicago. Prepared samples, collected and analyzed data.
- (2) Measurements of Basalt samples at room temperature and low temperature from M. Roskosz, Université de Lille 1. Collected and analyzed data.
- (3) Room temperature and low temperature measurements on superconducting FeTe film from Barry Wells, University of Connecticut. Collected and analyzed data.
- (4) Sample Characterization of Fe-bearing germanates under high pressure from Thomas Duffy, Princeton University. Collected and analyzed data.
- (5) Characterizing samples of Gd₁₃Fe₁₀C₁₃ and its Oxycarbide from D. C. Fredrickson, University of Wisconsin, Madison. Collected and analyzed data.
- (6) Mossbauer measurements of magnetoresistant samples (CaCu₃Fe₂Os₂O₁₂, Sr₂FeCrO₆, and Ca₂FeCrO₆) at room temperature and low temperatures. Collected and analyzed data.
- (7) Characterization of Li-ion battery materials from Chemical Science and Engineering, ANL. Collected and analyzed data.

- (8) Sample characterization of olivine samples from Jay Bass's group. Collected and analyzed data.

For educational outreach, I have organized and chaired the Nuclear Resonant Scattering Workshop on Nov. 7-9, 2014 at the APS, ANL. The workshop was organized as part of the OMPRES Education, Outreach and Infrastructure Development Programs to promote the application of the state-of-art Nuclear Resonant Scattering techniques for characterizing the properties of materials under the high P-T conditions of planetary interiors. Introductory lectures were offered by invited speakers and sector 3 beamline staff. Softwares CONUSS, PHOENIX and SciPhon for data evaluation were introduced and hands-on trainings were offered in the use of softwares. New features of the softwares and recent experiment capability developments were covered. The workshop attracted 39 participants from 15 institutions and 4 countries with various backgrounds of geosciences, physics, chemistry, material science and biophysics.

Beamtime Proposals I have involved in writing:

- (1) Development of High-Pressure and Low-Temperature Nuclear Resonant Scattering Capability for Geoscience and Condensed Matter Physics Applications at 3-ID (PUP-38969)
- (2) Origin of Jahn-Teller distortion and high-low spin transition of Fe_2TiO_4 , and FeCr_2O_4 and their pressure-induced structure transformation (GUP-32556)
- (3) Synchrotron Mössbauer Spectroscopy (SMS) Studies of the Magnetic State in Dy under Extreme Pressure (GUP-40395, self-PI)
- (4) Single Crystal X-ray Diffraction in EuFe_2As_2 under High Pressure (GUP-40428, self-PI)
- (5) The high pressure phonon density of states of fcc iron hydride (GUP-40453)

Education, Outreach, Workshop and Community service:

- (1) Organized and chaired the *Nuclear Resonant Scattering Workshop*, Nov. 7-9, 2014, APS, ANL.
- (2) Helped users to install CONUSS and PHOENIX software packages on their computers; trained new users from U. Hawaii, University of Texas at Austin, University of Illinois at Urbana-Champaign, Aarhus University (Denmark), Arizona State University and University of Chicago on how to use these softwares for data analysis.
- (3) Prepared and submitted proposal to Infrastructure Development programs of COMPRES titled "High pressure Low temperature Nuclear Resonant Scattering for Studying Properties of Planetary Materials in Extreme Environments. The proposal was awarded \$40,331 towards purchase of equipment for the project.
- (4) Prepared and submitted the 2-year- Partner User Proposal (PUP-38969) titled "*Development of High-Pressure and Low-Temperature Nuclear Resonant Scattering Capability for Geoscience and Condensed Matter Physics Applications at 3-ID*". The proposal was approved of 10% of 3-ID beamtime over 2 years.

- (5) Prepared and submitted the proposal of Workshop on Nuclear Resonant Scattering and Data Analysis to COMPRES Education & Outreach Programs. The proposal was approved to support the Workshop which was held on Nov. 7-9, 2014 at the APS, ANL.

List of recent publications and manuscripts in preparation

W. Bi, J. Zhao, J. Fu, Q. Jia, E. E. Alp, M. Y. Hu, X. C. Wang, C. Jin, R. Ferry, W. Yang, and V. Struzhkin, *Nuclear Resonant Inelastic X-ray Scattering at High Pressure and Low Temperature* (submitted to *Journal of Synchrotron Radiation*)

W. Bi, J. Lim, G. Fabbri, J. Zhao, D. Haskel, E. E. Alp, and J. S. Schilling, *Unusual Magnetism in Europium under 1 Mbar Pressure* (in preparation)

H. Liu, J. S. Tse, M. Y. Hu, **W. Bi**, J. Zhao, E. E. Alp, M. Pasternak, and R. D. Taylor, *Mechanism for Pressure-induced Amorphization of SnI_4* (submitted for publication)

M. Roskosz, C. K. I. Sio, N. Dauphas, **W. Bi**, F. L. H. Tissot, M. Y. Hu, J. Zhao and E. E. Alp, *Spinel-Olivine Iron Isotopic Thermo-oxybarometer Derived from NRIXS spectroscopic Measurements* (in preparation)

Bin Chen, Zeyu Li, Dongzhou Zhang, Jiachao Liu, Michael Y. Hu, Jiyong Zhao, **Wenli Bi**, E. Ercan Alp, Yuming Xiao, Paul Chow, and Jie Li, *Hidden carbon in Earth's inner core revealed by shear softening in dense Fe_7C_3* , PNAS (2014)

S. R. Bruno, C. K. Blakely, J. B. Clapham, J. D. Davis, **W. Bi**, E. E. Alp, and V. Poltavets, *Synthesis and Electrochemical Properties of Novel LiFeTiO_4 and $\text{Li}_2\text{FeTiO}_4$ Polymorphs with the CaFe_2O_4 -type Structures*, Journal of Power Sources, 273, 296 (2014)

A. B. Hadler, V. J. Yannello, **W. Bi**, E. E. Alp and D. C. Fredrickson, *$\text{Gd}_{13}\text{Fe}_{10}\text{C}_{13}$ and its Oxy carbide: Tracing Multiple Bonding and Oxygen Substitution in Carbometalates to the 18 electron rule*, JACS, 136, 12073 (2014)

M. K. Karunananda, E. E. Alp, **W. Bi**, S. Chattopadhyay, T. Shibata, and N. P. Mankad, *Experimental Determination of Metal-Metal Redox Cooperativity and Electronic Structure in Catalytically Active Cu-Fe and Zn-Fe Heterobimetallic Complexes*, Dalton Transactions, 43, 13661 (2014)

Jin Liu, Jung-Fu Lin, Ahmet Alatas, and **Wenli Bi**, *Sound Velocities of bcc-Fe and $\text{Fe}_{0.85}\text{Si}_{0.15}$ Alloy at High Pressure and Temperature*, Earth and Planetary Science Letters, 233, 24 (2014)

C. K. Blakely, J. D. Davis, S. R. Bruno, M. Zhu, X. Ke, **W. Bi**, E. E. Alp, and V. V. Poltavets, *Multistep Synthesis of the SrFeO_2F Perovskite Oxyfluoride via the SrFeO_2 Infinite-layer Intermediate*, Journal of Fluorine Chemistry, 159, 814 (2014)

S. Couet, H. Peelaers, M. Trekels, K. Houben, M.Y. Hu, J. Y. Zhao, **W. Bi**, E. E. Alp, E. Menéndez, B. Partoens, F. M. Peeters, M. J. Van Bael, A. Vantomme, and K. Temst, *Interplay Between Lattice Dynamics and Superconductivity in Nb_3Sn Thin Films*, Phys. Rev. B 88, 045437 (2013)