**IXS at High Pressure at 3-ID & Mössbauer Spectroscopy Lab of the APS**

2015 COMPRES Annual Report

Ercan Alp, Jiyong Zhao, Michael Hu, Ahmet Alatas, Thomas Toellner, ANL-APS

J. Bass, and Wenli Bi, UIUC

Total number of shifts requested:

In 2015 3-ID received 30 high-pressure-related proposals. Each proposal typically requests 5 days or 15 shifts, once or twice/year. So the total number of shifts requested is around 600.

Total number of shifts granted

In 2015, 18 proposals were allocated beamtime for high-pressure related research. Total number of shifts was 269.

Total number of shifts available

The General User Baseline is 200 shifts/cycle, or 600 shifts/year. After maintenance (8 %) is subtracted, the remaining 80 % is eligible for GUP time. So the total number of available shifts is 440. Of this, about 30 % is expected to be allocated for high-pressure research, which is 132. However, due to large demand this year, some of the internal time (which amounts to 110 shifts), and part of the maintenance periods, we were able to allocate more shifts to high-pressure experiments. Presence of PUP (J. Bass), and 5 scientists at 3-ID being themselves interested in high pressure experiments (E. Alp. A. Alatas, J. Zhao, M. Hu, and W. Bi) resulted in this increase. Recently, the quality and quantity of high-pressure proposals submitted, particularly those with an Earth science theme, have been such that they have received significantly more than the 30% target of beamtime.

(note that 3-ID has three main scientific application areas: High-pressure physics & Chemistry, Bioinorganic chemistry and Materials Science/Condensed matter physics)

Oversubscription rate (= shifts requested / shifts available)

The oversubscription rate for high pressure related experiments at 3-ID is 3-to-4 times.

Number of visits by distinct research groups in 2015

Number of distinct research groups: 11:

PI Institution No. of Shifts

Jay Bass & Wenli Bi UIUC, 54 (PUP)

Afu Lin, UT Austin, 71

Shun Ichiro Karato, Yale: 6

Andrew Campbell, U Chicago 9

Nicolas Dauphas, U Chicago 18

Bin Chen U Hawaii 15

Wenli Bi UIUC-Compres 18

E. Alp ANL 21

Jennifer Jackson Caltech 27

John Tse U. of Saskatchewan 15

M. Pasternak Tel Aviv University 15

Conventional Mössbauer Spectroscopy facility at the APS

* Which publications resulted from the conventional Mossbauer, and which from the synchrotron beamline?

Mössbauer measurements are typically done for characterizing samples before and after the experiments. In other words, they are embedded, sometimes in the main paper, sometimes in the supporting information, and sometimes not at all.

The measurements are based upon a simple request. A graduate student, postdoct or professor can ask for a measurement. We discuss the sample requirements, and perform the measurement. Typically, we will also fit the data and provide guidance on interpretation. There is no formal proposal procedure. If measurement is feasible, we will do it.

The Mössbauer facility has been advertised to the COMPRES community via COMPRES annual meetings presentations (oral and poster), as well as via users coming to the APS.

List of publications that made use of data taken at the Mössbauer Lab (2015):

Amelia B. Hadler, Vincent J. Yannello, Wenli Bi, E. Ercan Alp, and Daniel C. Fredrickson

, “π‑Conjugation in Gd13Fe10C13 and Its Oxycarbide: Unexpected Connections between Complex Carbides and Simple Organic Molecules, J. Am. Chem. Soc. 2014, 136, 12073−12084

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,"](http://dx.doi.org/10.1016/j.gca.2015.07.035) Geochim. Cosmochim. Acta 169, 184-199 (2015).

M. Blanchard, N. Dauphas, M.Y. Hu, M. Roskosz, E.E. Alp, D.C. Golden, C.K. Sio, F.L.H. Tissot, J. Zhao, L. Gao, R.V. Morris, M. Fornace, A. Floris, M. Lazzeri, E. Balan, ["Reduced partition function ratios of iron and oxygen in goethite,"](http://dx.doi.org/10.1016/j.gca.2014.12.006) Geochim. Cosmochim. Acta 151, 19-33 (2015

Karunakar Kothapalli, Eunja Kim, Tomasz Kolodziej, Philippe F. Weck, Ercan E. Alp, Yuming Xiao, Paul Chow, C. Kenney-Benson, Yue Meng, Sergey Tkachev, Andrzej Kozlowski, Barbara Lavina, Yusheng Zhao, ["Nuclear forward scattering and first-principles studies of the iron oxide phase Fe[subscript 4]O[subscript 5],"](http://dx.doi.org/10.1103/PhysRevB.90.024430) Phys. Rev. B 90 (2), 024430-1-024430-5 (2014).

Bin Chen, Zeyu Li, Dongzhou Zhang, Jiachao Liu, Michael Y. Hu, Jiyong Zhao, Wenli Bi, E. Ercan Alp, Yuming Xiao, Paul Chow, Jie Li, ["Hidden carbon in Earth's inner core revealed by shear softening in dense Fe[subscript 7]C[subscript 3],"](http://www.pnas.org/content/111/50/17755) Proc. Natl. Acad. Sci. USA 111 (50), 17755-17758 (2014).

N. Dauphas, M. Roskosz, E.E. Alp, D.R. Neuville, M.Y. Hu, C.K. Sio, F.L.H. Tissot, J. Zhao, L. Tissandier, E. Médard, C. Cordier, ["Magma redox and structural controls on iron isotope variations in Earth’s mantle and crust,"](http://dx.doi.org/10.1016/j.epsl.2014.04.033) Earth Planet. Sci. Lett. 398, 127-140 (2014).

Colin K. Blakely, Joshua D. Davis, Shaun R. Bruno, Shannon K. Kraemer, Mengze Zhu, Xianglin Ke, Wenli Bi, E. Ercan Alp, Viktor V. Poltavets, ["Multistep synthesis of the SrFeO[subscript 2]F perovskite oxyfluoride via the SrFeO[subscript 2] infinite-layer intermediate,"](http://dx.doi.org/10.1016/j.jfluchem.2013.12.007) J. Fluorine Chem. 159, 8-14 (2014).

List of users of the conventional Mossbauer system (2014-2015)

* **Jay Bass,** University of Illinois Urbana-Champaign
* **Wenli Bi,** University of Illinois Urbana-Champaign/Argonne
* **Thomas Duffy,** Princeton University
* **Jennifer Jackson**, Caltech
* **Shun-ichiro Karato**, Yale University
* **Sang-Heon Dan Shim**, Arizona State University
* **Jung-Fu Lin**, University of Texas at Austin
* **Nicolas Dauphas**, University of Chicago
* **Mathieu Roskosz,** Université de Lille I, France
* **Takamitsu Yamanaka,** Geophysical Lab., Carnegie Institution of Science
* **Susannah Dorfman**, Michigan State University
* **Christy Till**, Arizona State University
* **Przemek Dera**, University of Hawaii
* **Bin Chen,** University of Hawaii
* **Barbara Lavina,** University of Nevada, Las Vegas
* **Michael Krawcyznski,** Washington University in St. Louis
* **Andrew Campbell,** University of Chicago
* **Mathieu Roskosz,** Université de Lille I, France
* **Barbara Lavina,** University of Nevada, Las Vegas
* **Viktor Struzhkin,** Geophysical Laboratory, Carnegie Institution of Science
* **Caitlin Murphy,** Geophysical Laboratory, Carnegie Institution of Science
* David Harris, Northwestern University
* Daniel Frederickson, University of Wisconsin