

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, postdoc 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," 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," 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 Kozłowski, Barbara Lavina, Yusheng Zhao, "Nuclear forward scattering and first-principles studies of the iron oxide phase Fe_4O_5 ," 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_7C_3 ," 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," 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_2F perovskite oxyfluoride via the SrFeO_2 infinite-layer intermediate," 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 Krawczynski**, 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

Mark Rivers

From: Mark Rivers
Sent: Sunday, December 20, 2015 5:09 PM
To: Alp, Esen E.; 'wbi@aps.anl.gov'; Bass, Jay D
Cc: Jackson, Jennifer M.; Carl Agee; Andrew Campbell; Chen, Bin; Dan Shim; Kanani Lee; Bass, Jay D
Subject: RE: COMPRES annual report for Sector 3-ID activities

Dear Ercan, Wenli, and Jay,

We discussed your report at the meeting of the COMPRES Facilities and Executive Committees this week. Both groups wished to have some more information. Our report request specifically asked for the following information in the template file:

- Total number of shifts requested
- Total number of shifts granted
- Total number of shifts available
- Oversubscription rate (= shifts requested / shifts available)
- Number of visits by distinct research groups

Please include the above information for all groups, and also specifically for the COMPRES groups.

We would also like the following information:

- Please identify the PIs of this project on the first page of the report.
- For the conventional Mossbauer system please provide the following information:
 - Which publications resulted from the conventional Mossbauer, and which from the synchrotron beamline?
 - Explain how beam time on the conventional Mossbauer system is allocated.
 - Provide a list of users of the conventional Mossbauer system
 - Explain how the conventional Mossbauer system has been advertised or will be) to the COMPRES community.

We would like to receive your response by January 5.

Thanks,
Mark

From: Alp, Esen E. [eea@aps.anl.gov]
Sent: Friday, November 06, 2015 11:35 AM
To: Mark Rivers
Cc: Jackson, Jennifer M.; Carl Agee; Andrew Campbell; Chen, Bin; Dan Shim; Kanani Lee; Bass, Jay D
Subject: COMPRES annual report for Sector 3-ID activities

Hi, Mark:

Attached please find a revised and complete version of our contribution to COMPRES 2015 annual report, as well as Dr. Wenli Bi's activity report.

Thanks for your understanding of the special circumstances. We also want to thank Jay Bass for his critical reading.

Mark Rivers

From: Alp, Esen E. <eea@aps.anl.gov>
Sent: Tuesday, January 05, 2016 4:34 PM
To: Mark Rivers
Subject: 3-ID and Mossbauer lab addendum to COMPRES Annual report
Attachments: COMPRES Annual Report_MossbauerLab_2015.docx

Dear Mark:

Please find our response to your questions. I had a difficult time to complete your questions regarding the Mossbauer facility in the lab.

Some of the papers listed made use of the Mossbauer Lab data at either an earlier stage, or later stage of the experiments conducted at the beamline. Very few acknowledged COMPRES support for the facility, due to our failure to remind the users to do so. This is something we can do from now on.

Please let us know if this is adequate, or I can work on the issues you might have.

Best regards

Ercan-Wenli-Jay

Mark Rivers

From: Mark Rivers
Sent: Tuesday, January 05, 2016 5:00 PM
To: 'Alp, Esen E.'
Subject: RE: 3-ID and Mossbauer lab addendum to COMPRES Annual report

Hi Ercan,

Thanks for sending that. I had a few questions about it.

The text says that 269 shifts were allocated to high pressure, but the sum of the shifts in the table is 219. Which is correct?

You said: "Of this, only 30 % is available for high-pressure research, which is 132."

But high-pressure actually received more than this, either 219 or 269? What is the meaning of the 30% number?

Is your list of users of the conventional Mossbauer system for this reporting year, or cumulative since it began? Can you identify who used it in this reporting year?

Thanks,
Mark

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Sent: Tuesday, January 05, 2016 4:34 PM
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Best regards

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From: Alp, Esen E. <eea@aps.anl.gov>
Sent: Wednesday, January 06, 2016 2:08 PM
To: Mark Rivers
Cc: Bi, Wenli; Jay Bass; Zhao, Jiyong
Subject: Re: 3-ID and Mossbauer lab addendum to COMPRES Annual report
Attachments: COMPRES Annual Report_MossbauerLab_2015.docx

Hi, Mark

Thanks for pointing out the inconsistency in the numbers given in the table and text. I had undercounted the beam time given to PUP (Bass) and Afu Lin, who also used 3-ID-C beamline for IXS measurements. The numbers are now consistent.

The meaning of 30 % is our general desire to maintain a balance between 1) high-pressure/geophysics experiments, 2) biophysics/bioinorganic chemistry and 3) materials science/condensed matter physics experiments. In the last 20 years, we maintained a rough balance between these programs, with the goal of expanding the applications of inelastic and nuclear resonant scattering into widest possible research fields. However, due to large demand this year, some of the internal time (which amounts to 110 shifts), and maintenance periods were allocated 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 this increase.

As for publications, I have now only included 2015 papers.

Best regards, and good luck with the report.

Ercan

On Jan 5, 2016, at 4:59 PM, Mark Rivers <rivers@cars.uchicago.edu> wrote:

Hi Ercan,

Thanks for sending that. I had a few questions about it.

The text says that 269 shifts were allocated to high pressure, but the sum of the shifts in the table is 219. Which is correct?

You said: "Of this, only 30 % is available for high-pressure research, which is 132."

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Mark Rivers

From: Mark Rivers
Sent: Wednesday, January 06, 2016 2:16 PM
To: 'Alp, Esen E.'
Cc: Bi, Wenli; Jay Bass; Zhao, Jiyong
Subject: RE: 3-ID and Mossbauer lab addendum to COMPRES Annual report

Hi Ercan,

Sorry, can I ask you to make 2 more changes.

- Include 2014 publications for consistency with other reports. Some of the 2014 publications may have come since your 2014 report that was submitted in October 2014.
- Indicate which users of the conventional Mossbauer used it in 2014 or 2015.

I promise I won't ask for anything else!

Thanks,
Mark

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From: Alp, Esen E. <eea@aps.anl.gov>
Sent: Wednesday, January 06, 2016 2:38 PM
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Cc: Bi, Wenli; Jay Bass; Zhao, Jiyong
Subject: Re: 3-ID and Mossbauer lab addendum to COMPRES Annual report
Attachments: COMPRES Annual Report_MossbauerLab_Final_2015.docx

Dear Mark:

No problem at all answering your questions. I have now included 2014 publications. The users listed there were indeed people who used the facility during the last two years. No changes are required.

Best regards

Ercan

On Jan 6, 2016, at 2:15 PM, Mark Rivers <rivers@cars.uchicago.edu> wrote:

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Sent: Wednesday, January 06, 2016 5:08 PM
To: Mark Rivers
Cc: Jay Bass; Bi, Wenli
Subject: A better version
Attachments: COMPRES Annual Report_MossbauerLab_Final_2015.docx

Dear Mark:

I you have not yet incorporated the last version I had sent you, please use this version instead. Jay Bass had some corrections, and I have now had a chance to include them. Relatively minor but relevant corrections were made.

Thanks

Ercan