ALS Beamline 12.2.2
2016 COMPRES Annual Report
November 2015 – November 2016
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Overview/Personnel/Management

The operations at beamline 12.2.2 have had a highly successful last year: our personnel on both the COMPRES and ALS side have formed a cohesive ongoing team, comprised of COMPRES funded staff members Christine Beavers and Jinyuan Yan, and ALS funded personnel Martin Kunz and Andrew Doran. Beamline Manager Alastair MacDowell, who played a primary role on the ALS side in managing 12.2.2 from 2010-14 continues to be formally allocated partly to 12.2.2, but the present staffing by the 12.2.2 team has reduced the need for his high-level expertise and management largely to advice on highly complex beamline issues, often associated with x-ray optics. Our publication output is healthy and increasing, and our accessing of beamtime by COMPRES-related users runs between 50 and 62% of the available time in each cycle, which is well in excess of the 35% guaranteed under the COMPRES Approved Program agreement with ALS management. Our sample preparation infrastructure continues to be excellent (and our sample preparation facility was substantially reorganized in the past year to enhance both space utilization and safety), with our gas-loading system and laser miller each being used extensively by users. In this report, we emphasize new developments which include: our new single crystal x-ray diffraction system becoming operational, continued work on external heating at high pressures, and work on two-sided laser-heated radial diffraction. In passing, we note that 12.2.2 and its infrastructure have also functioned as a support facility for the high-pressure infrared set-up from NSLS that has been deployed by Zhenxian Liu at beamline 1.4.3. This support takes various forms, from 12.2.2 somewhat functioning as the Orchard Supply Hardware for the new set-up at 1.4.3 (as in “Hey!! Did that optical breadboard grow legs and walk over here from 12.2.2?”) to usage by IR users (to date, Liu, Campbell group, and Williams group) of our sample prep facilities and our ruby fluorescence system. It’s all good, and we’re happy to help with the nascent IR effort, particularly as folks can now (in concept) do nearly simultaneous IR and XRD measurements at the ALS, which is a potentially very valuable paired capability to offer the community.

Scientific Highlights

We continue to maintain and augment our state-of-the-art radial diffraction capabilities, and these were recently deployed to produce a high-profile study of texturing across the zircon to scheelite transition (Yue, Hong, Merkel, Tan, Yan, Chen and H.K. Mao, PRL, 117, 135701, 2016). The results, shown in Fig. 1, clearly demonstrate the long-inferred topotactic nature of this transition, in which the texture in the 001 direction in zircon transforms into the 110 direction in scheelite. These results illustrate the capability of our system to reliably characterize the texture of complex materials as they undergo phase transitions—a key capability for determining deformational characteristics of coexisting phases, and characterizing mechanisms of phase transitions.

There is an ulterior motive behind presenting this result, beyond it being interesting and high-profile. This contribution illustrates an ambiguity that will show up later in this report that is produced in the process of assessing the various forms of the query posed by the Facilities Committee of "how much time is allocated to COMPRES" at the ALS. This study (on a mineral analogue system) was led by HPSTAR scientists, in collaboration with both some reasonably well-known members of the high-pressure geosciences community (S. Merkel and H.K. Mao) and a COMPRES-funded scientist (Yan). It also (very appropriately) acknowledges COMPRES support. However, as near as we can tell from the COMPRES website, HPSTAR isn't a COMPRES member (perhaps this has changed, and the website is out-of-date?). So, the question arises: do we count the time used for this study as COMPRES time? If we counted from a pure institutional-affiliation-with-COMPRES perspective, the answer might be no, which seems downright peculiar. This seemingly semantic issue is of interest for our statistics, as HPSTAR has a Cooperative Agreement that guarantees it 10% of the time at 12.2.2, and they are often supported in this time by COMPRES scientists.

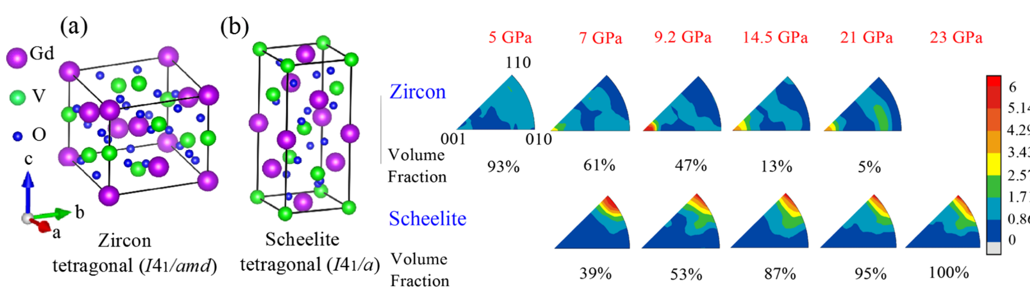

Figure 1. Structures and textural evolution of zircon and scheelite, as measured by radial diffraction at 12.2.2. From Yue et al., PRL, 2016.

Our second highlight illustrates our developing single-crystal capabilities. Here, hybrid perovskites are probed at relatively modest pressures (Jaffe, Lin, Beavers, Voss, W.L. Mao and Karunadasa, ACS Central Science, 2, 201-209, 2016). Because of the complexity and high compressibility of these materials $(CH_3NH_3)PbBr_3$ and $(CH_3NH_3)PbI_3$), marked structural changes occur at modest pressures: these shifts in symmetry are readily recognized within the mineral physics community, and the robustness of the octahedral tilting of perovskites across such a large range of chemical substituents provides a stark reminder of the ubiquity of the concepts probed by the high-pressure geosciences community. The materials science rationale for these studies lies in the possible technological usages of these inorganic-organic hybrid semiconductors in applications ranging from solar cell absorbers to light emitting diodes. Nevertheless, we highlight this example as illustrating our developing capabilities at resolving relatively complex structures under pressure at 12.2.2.

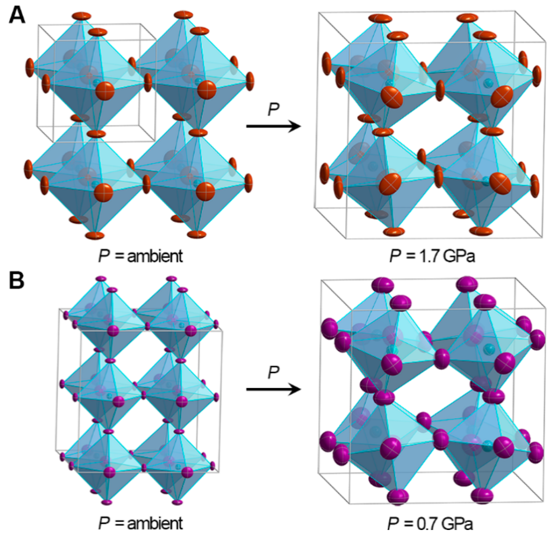

Figure 2. Single-crystal structures of $(CH_3NH_3)PbBr_3$ (A) and $(CH_3NH_3)PbI_3$ (B). Turquoise, purple and brown thermal ellipsoids represent Pb, I and Br atoms, respectively: the organic portion in the big site is omitted for clarity.

Overview of Developments: (1) High Pressure Single Crystal: A Maturing Capability

The single crystal high pressure program continues to grow and evolve towards a mature state, led by COMPRES employee Christine Beavers. By spring 2017, each endstation on beamline 12.2.2 will offer single crystal diffraction data collection capabilities, with advantages to each. Endstation 1(ES1), which is collecting data now but for which some of the mechanical features remain to be completed, offers a 4-circle STOE diffractometer with a 10 micron sphere of confusion, and the capability to carry BX90 DACs (engineered in a collaboration between STOE and 12.2.2: the manufacturer's blurb on our facility can be seen at: https://www.stoe.com/advanced-light-source-selects-stoe-stadivari-diffractometer-the-most-precise-four-circle-xrd-for-single-crystal-high-pressure-research/). We expect that ES1 will be fully available to general users in spring 2017. One of our primary goals, and design principles, for this system is to make synchrotron-based high-pressure single-crystal experiments far more routine for users (and particularly users that are not crystallography aficionados) than has typically been the case. In terms of our hardware, the Stoe Stadi-Vari 4-circle diffractometer equipped with an RDI CMOS fast detector was purchased by the ALS in fall 2015 (the diffractometer was $181 K from ALS/DOE funding, and the CMOS detector was also ALS funded at $75 K: these were, of course, partially leveraged by COMPRES' commitment to this beamline). The diffractometer was installed in spring 2016 on a temporary three-point mount, to allow for rough alignment and system optimization. COMPRES awarded funds from its EOID program ($85 K) to purchase robust stages (and a custom collimator) to accurately position the diffractometer on the beam focus point in spring 2016; these stages have now arrived, and will be installed during beam down-time in December 2016. These stages, along with the COMPRES-funded adjustable collimator, will complete the single crystal apparatus on ES1.

And, in recent excellent developments, the ALS has agreed (as of 8/16) to fund a large format CMOS detector to augment the detector options on beamline 12.2.2: this detector, which will cost **north of $200 K**, is partially envisioned as an improved replacement for our older MAR detector. As such, the ALS will have invested in equipment alone (renovations, which were far from free, also had to be conducted at 12.2.2 to enable the mounting of the diffractometer on ES1) $450-K-ish of their money to equip 12.2.2 in the last two years; COMPRES will have put in $85 K and, of course, the staffing and user community that enables the COMPRES/ALS partnership.

Endstation 2, which is currently operational, offers less angular range, but can support large DACs on its single rotation axis. The single crystal program on both endstations is built around high-speed, shutter-less detectors, and offers users the ability to finely slice reciprocal space in a timely manner, leading to more accurate intensities and higher precision on lattice parameters. ES2 continues to produce impressive data, despite the low percentage of reciprocal space that can be accessed. The Huber stages and rotation axis employed in ES2 were factory refurbished in early 2016 (again at ALS expense), to ensure their continued performance. The Perkin Elmer detector, which has been controversial among users because of the noisy nature of its images, is now understood well enough to analyze the resulting data properly: this improved understanding allows for structure solutions and high quality refinements of reasonably complex systems on this end-station.

Overview of Developments (2): Development Work on Resistive and Laser Heating

As part of the development of 12.2.2's portfolio of high pressure and a broad suite of high temperatures, we have continued (through Jinyuan Yan) our developmental work on resistive heating during the review period. Ultimately, the plan here is, of course, to dovetail our SCXRD developments with improved, compact, efficient resistive heating to routinely access temperatures above (and hopefully substantially above) 1000 K. In the past, we (led by Lowell Miyagi) have deployed a graphite heater to heat a diamond cell to over 1700 K, but the setup and sample loading of these systems are time-consuming, and they have very low success rates: they are heroic experiments. Simpler external heaters are easily setup, but are seldom deployed above 1000-1100 K. We have in development a novel tungsten external heater for the modified BX90 cell, for which we have achieved temperatures up to 1685 K when buffered with reducing gas. However, maintaining the pressure at these high temperature conditions has proved challenging: our current step in this project is to shift components/the thermal conditions on the exterior of the cell to minimize the loss of pressure while heating. This heater is designed to be a modular, plug-and-play design and is hence quite user friendly. It covers both the low temperature range, and also (critically) overlaps the higher temperature range that is achievable by laser heating.

In tandem with the external heating project, we are also taking advantage of our recently rebuilt laser-heating system (last annual report) to institute double-sided laser heating for radial diffraction experiments. There have been geometric limitations associated with such experiments, including difficulties with laser de-focusing during heating. A new double-sided system has been designed that is currently undergoing testing.

In terms of community development/outreach, once the hardware of our high-pressure single crystal set-up is finalized and the software is fully shaken out, we plan to run a community workshop on the experimental ease of high-pressure single-crystal diffraction measurements, focused on non-expert users. Otherwise, beamline folks have heavily promoted the beamline at several crystallography meetings in the last 18 months (including ACA and the European Crystallography meeting), as well as COMPRES and AGU.

So, to conclude, this represents a snapshot of the new areas we are pursuing/finalizing this coming year, and the new equipment that we have leveraged by strategically deploying the COMPRES investment at the Advanced Light Source.

Beamline Operations

(1) Number of beamtime proposals received
Cycle 1-2016: 63 (+1 AP)HP*)), ~ 26 of which are COMPRES
Cycle 2-2016: 50 (+2 AP's), 26 COMPRES

(2) Number of beamtime proposals granted beamtime
Cycle 1-2016: 22, 11 COMPRES
Cycle 2-2016: 28, 13 COMPRES

(3) Total number of shifts requested
Cycle 1-2016: 501 (+ 29 HP*), 217 COMPRES (w/o HPSTAR; 245 w/HP*)
Cycle 2-2016: 423 (+50 AP's), 219 COMPRES

(4) Total number of shifts granted
Cycle 1-2016: 215 (incl HP*), 117 or 137 (with HPSTAR) COMPRES (includes Director's Discretionary Time)
Cycle 2-2016: 261 (incl AP's), 163 COMPRES, or 183 (with HPSTAR)

(5) Total number of shifts available
Cycle 1-2016: as (4): 215
Cycle 2-2016: as (4): 261

(6) Oversubscription rate (= shifts requested / shifts available)
Cycle 1-2016: 2.46 (1.85 COMPRES)
Cycle 2-2016: 1.81 (1.34 COMPRES)

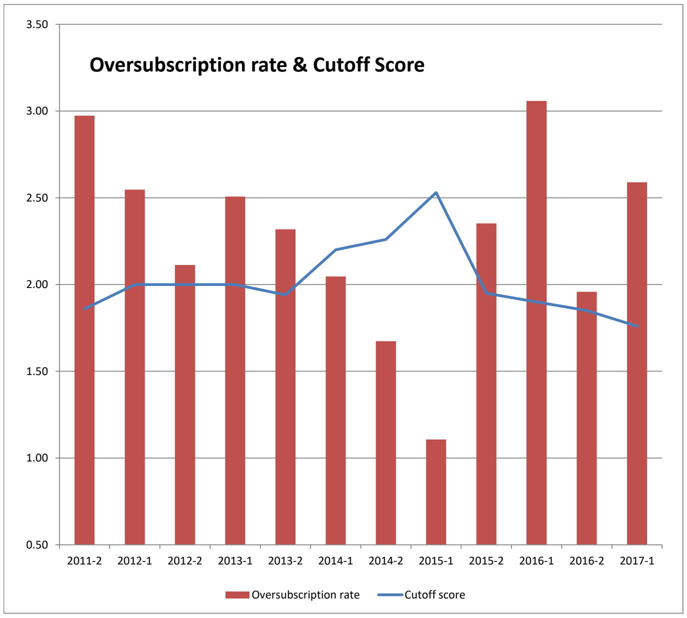

Figure 3. Oversubscription and Cutoff scores for 12.2.2. Proposals are rated on a 1-5 scale, with 1 being the highest and 5 being the lowest. For reference, 2015-1 was the cycle in which the ALS User office shifted their PI notification policies in stealth mode: proposal PIs, who had always been sent personalized email reminders to resubmit their proposals, only received one generic "call for proposals" email. This change had an amazing impact that was not recognized until after the proposal deadline, and a dramatic dip in proposals was an around-the-ring phenomenon. Needless to say, this change was reversed for the following cycle.

Performance Metrics

In the Nov 2015- present span, we had 26 distinct research groups visit the ALS to use 12.2.2 in 63 different visits. The funding sources and days allocated for these groups are listed in the performance metrics section. Our user office reports that we had visits from 82 badged users, comprised of 12 faculty, 36 GSRA, 15 post-docs, 14 scientists/technical staff, and 5 undergrads. Person visits, as we understand them, are less straightforward to track (especially for local groups, a shifting cast of characters shows up at different times), but our estimate is that we had about 140 person visits.

COMPRES users made up 58% of allocated shifts over the course of Nov 2015-Nov 2016 if HPSTAR usage is included in the COMPRES count; and 47.7% without HPSTAR. In either case, this far exceeds the mandated 35% dictated by the COMPRES AP.
The table below shows the different groups, their time allotments, their country, and their funding sources over the last year. These are subdivided into the three beamtime cycles that are spanned by the report period.

ALS 12.2.2	ALS 12.2.3	ALS 12.2.4	ALS 12.2.5	ALS 12.2.6	ALS 12.2.7	LS 12.2.	LS 12.2.	LS 12.2.1	LS 12.2.1	S 12.2.	LS 12.2.1	LS 12.2.1	LS 12.2.1
PI Name	# days	Beam time	COMPRES User ©	Funding Source	Country	NSF-EAR	NSF-DMR	NSF-Chem	DOE	DOD	NSF-China	NNSA	Foreign
ALS on Shutdown	--	11/1/15- 1/15/16											
McCluskey	1.66	1/16-1/17		NSF-DMR	USA		1						
Willams	1	1/21-1/22	C	NSF-EAR	USA	1							
Santamaria-Perez	3	1/22-1/25	C	Foreign (NSF)/NSF-EAR	Spain/USA	1							1
Jeanloz	2	1/26-1/28	C	DOE	USA				1				
Bin Chen(Hi)	3.66	1/28-1/31	C	NSF-EAR	USA	1							
85.3% COMPRES	11.32		80.00%										
	2016-1	1/1/16-6/30/16											
PI Name	# days	Beam Time											
Alivisatos	4	4/5-4/6; 5/13-5/16		DOE-MSE	USA				1				
Bin Chen(HP*)	6.66	3/30-4/2; 5/26-5/29	C?	Foreign (NSF)	China						1		1
Chan	3	2/19-2/22		NSF-DMR	USA		1						
Ciezak-Jenkins	3	2/5-2/8		DOD	USA					1			
Ewing (Rittman)	3	6/24-6/27	C	NSF-EAR	USA	1							
Gilbert (Banfield)	4	3/2-3/6	C	DOE	USA				1				
Jackson	4	4/28-5/2	C	NSF-EAR	USA	1							
Kavner	2.66	4/8-4/10	C	NSF-EAR	USA	1							
Long	2	2/3-2/4; 6/23-6/24		NSF-Chem	USA			1					
Mattox	1	6/9-6/10		DOE	USA				1				
McCluskey	4.33	2/12-2/14; 5/21-5/22		NSF-DMR	USA		1						
Miyagi	4	5/4-5/8	C	NSF-EAR	USA	1							
Montiero	2	2/26-2/28		DOE	USA				1				
Olmstead	1	6/15-6/16		NSF-Chem	USA			1					
Ross	3.66	4/21-4/24	C	NSF-EAR	USA	1							
Santamaria-Perez	2	6/1-6/3	C	Foreign (NSF)/NSF-EAR	Spain/USA	1							1
Stavrou	2	6/3-6/5		NNSA/DOE	USA				1			1	
Tolbert	2.66	3/11-3/13	C	NSF-DMR	USA		1						
Wenk	3	6/28-7/1	C	NSF-EAR	USA	1							
Willams	6	2/18-2/19; 4/7-4/8; 4/27-4/28; 5/19-5/21; 5/25-5/26	C	NSF-EAR	USA	1							
Yaghi	3.66	2/4-2/5; 4/6-4/7; 6/18-6/19		DOE	China				1		1		1
51.7% COMP; 61.6% **	67.63		58.82%										
ALS 12.2.2	2016-2	7/1/2016-11/1/2016											
PI Name	# days	Beam Time											
Alivisatos	2	8/8-8/10		DOE-MSE	USA				1				
Bin Chen(HP*)	6.66	8/11-8/14; 10/20-10/23	C?	Foreign (NSF)	China						1		1
Ciezak-Jenkins	3	7/8-7/11		DOD	USA					1			
Gilbert/Banfield	2	10/12-10/14	C	DOE	USA				1				
Gurlo	5	9/29-9/30; 10/11-10/12; 10/15-10/16; 10/29-10/31		Foreign (NSF)	Germany								1
Liu	2	7/29-7/31	C	Foreign (NSF)	China						1		1
Long	1	7/20-7/21		NSF-Chem	USA			1					
McCluskey	2.66	9/9-9/11		NSF-DMR	USA		1						
Montiero	1	9/22-9/23		DOE	USA				1				
Olmstead	1	9/28-9/29		NSF-Chem	USA			1					
Santamaria-Perez	2	7/22-7/25	C	Foreign (NSF)/NSF-EAR	Spain/USA	1							1
Stavrou	3	9/16-9/19		NNSA/DOE	USA				1			1	
Tolbert	2.66	7/1-7/3	C	NSF-DMR	USA		1						
Tschauner	1.66	7/16-7/17	C	NSF-EAR/NNSA/DOE	USA	1			1			1	
Wenk	1	9/7-9/8	C	NSF-EAR	USA	1							
Willams	5	7/12-7/13;9/2-9/3; 9/20-9/22; 10/19-10/20	C	NSF-EAR	USA	1							
Yaghi	1.66	9/3-9/4		DOE	USA								
Zeng	5.66	9/30-10/2; 10/29-10/31	C	DOE/Foreign (NSF)	China/USA				1		1		
44.9% COMP; 58.5% **	48.96		50.00%	Totals	42	15	6	4	13	2	5	3	8
						34.09%	13.64%	9.09%	29.55%	4.55%	11.36%	6.82%	18.18%
						NSF-EAR	NSF-DMR	NSF-Chem	DOE	DOD	NSF-China	NNSA*	Foreign

*NNSA supported users were all also DOE supported
All time was allocated through the GU panel, with the exception of the HPSTAR and Gurlo Approved programs, which received 10% and 5%, repectively during their terms.
**COMPRES including HPSTAR

Table 1. Users, time allocations, COMPRES affiliations, and funding sources.

List of Users (Group Leaders) with Affiliations 11/1/15 to present:

A. Alivisatos (UCB Chemistry/LBNL)
C. Beavers (COMPRES)
J.M. Brown (U. Washington: Director's Discretionary Time)
B. Chen (Hawaii)
J. Ciezak-Jenkins (Aberdeen Proving Ground)
R. Ewing/ Rittman (Stanford)
B. Gilbert (LBNL/UCB: Banfield collaboration)
A. Gurlo (Ceramics, TU Berlin)
HPSTAR (Rotating cast of ~15 people)
J. Jackson (Caltech)
D. Jacob and S. Clark (Macquarie U.)
R. Jeanloz (UC Berkeley)
A. Kavner, including Santamaria-Perez time (UCLA)
M. Kunz (ALS)
W. Mao, including Zeng time (Stanford)

M. McCluskey (WSU Chemistry)
L. Miyagi (Utah)
P. Monteiro (UCB Materials Science)
M. Olmstead (UCD Chemistry)
N. Ross (Virginia Tech)
S.-H. Shim (ASU)
E. Stavrou (LLNL)
S. Tolbert (UCLA Chemistry)
H.R. Wenk (UC Berkeley)
Q. Williams, including O'Bannon and Yan time (UC Santa Cruz)
O. Yaghi (UCB Chemistry)

Appendix 1. COMPRES-Related 12.2.2 Publications from 10/15 (Last Annual Report) to 10/16*

*just FYI, we haven't included papers that don't involve COMPRES assistance and really have nothing to do with the COMPRES mission (those would be papers on highly energetic organic materials)—if you'd like those too, happy to include them.

(1) Bae, Youn Jue, Eun Seon Cho, F. Qiu, Daniel T. Sun, Teresa E. Williams, Jeffrey J. Urban, and Wendy L. Queen, "Transparent Metal–Organic Framework/Polymer Mixed Matrix Membranes as Water Vapor Barriers," ACS Applied Materials and Interfaces 8(16), 10098-1010 (2016). (doi:10.1021/acsami.6b01299)

(2) Chen, B., Jung-Fu Lin, Jiuhua Chen, Hengzhong Zhang, and Qiaoshi Zeng, "Synchrotron-based high-pressure research in materials science," Materials Research Society Bulletin 41(6), 473-478 (2016). (doi:10.1557/mrs.2016.110) 1.4,12.2.2,12.3.2

(3) Chen, Y., S. Zhang, W., Gao, F. Ke, J. Yan, B. Saha, C. Ko, B. Chen, J.W. Ager III, W. Walukiewicz, R. Jeanloz, and J. Wu, "Pressure-induced structural transition of $Cd_xZn_{1-x}O$ alloys," Applied Physics Letters 108(15), 152105 (2016). (doi:10.1063/1.4947022) 12.2.2

(4) Du, W., Simon Ma Clark, and David Walker, "Excess mixing volume, microstrain, and stability of pyrope-grossular garnets," American Mineralogist 101(1), 193-204 (2016). (doi:10.2138/am-2016-5128) 12.2.2

(5) Fan, W., X.i. Zhu, Feng Ke, Yabin Chen, Kaichen Dong, J. Ji, B. Chen, Sefaattin Tongay, Joel W. Ager, K. Liu, Haibin Su, and Junqiao Wu, "Vibrational spectrum renormalization by enforced coupling across the van der Waals gap between MoS_2 and WS_2 monolayers,"Physical Review B: Condensed Matter and Materials Physics 92(24), 241408 (2015). (doi:10.1103/PhysRevB.92.241408) 12.2.2

(6) Gilbert, B., L.R. Comolli, R.M. Tinnacher, M. Kunz, and J. Banfield, "Formation and restacking of disordered smectite osmotic hydrates," Clays and Clay Minerals 63(6), 432-442 (2015). (doi:10.1346/CCMN.2015.0630602) 12.2.2,12.3.2

(7) Gleissner, J., D. Errandonea, A. Segura, J. Pellicer-Porres, M. A. Hakeem, J. E. Proctor, S. V. Raju, R. S. Kumar, P. Rodríguez-Hernández, A. Muñoz, S. Lopez-Moreno, and M. Bettinelli, "Monazite-type $SrCrO_4$ under compression," Physical Review B: Condensed Matter and Materials Physics 94(13), 134108 (2016). (doi:10.1103/PhysRevB.94.134108) 12.2.2

(8) Hong, Fang, Binbin Yue, Zhenxiang Chen, Martin Kunz, B. Chen, and Ho-Kwang Mao, "High pressure polymorphs and amorphization of upconversion host material $NaY(WO_4)_2$,"Applied Physics Letters 109, 041907 (July 29 2016). (doi:10.1063/1.4960104) 12.2.2

(9) Jaffe, A., Y.u. Lin, C.M. Beavers, Johannes Voss, Wendy L. Mao, and H.I. Karunadasa, "High-Pressure Single-Crystal Structures of 3D Lead-Halide Hybrid Perovskites and Pressure Effects on their Electronic and Optical Properties," ACS Central Science 2(4), 201-209 (2016). (doi:10.1021/acscentsci.6b00055) 11.3.1,12.2.2

(10) Lech, Andrew T., Christophe Turner, Jialin Lei, Reza Mohammadi, Sarah H. Tolbert, and Richard B. Kaner, "Superhard Rhenium/Tungsten Diboride Solid Solutions," Journal of the American Chemical Society 138(43), 14398-1440 (2016). (doi:10.1021/jacs.6b08616) 12.2.2

(11) Liu, Gang, Lingping Kong, Jinyuan Yan, Zhenxian Liu, Hengzhon Zhang, P. Lei, T. Xu, Ho-kwang Mao, and B. Chen, "Nanocrystals in compression: unexpected structural phase transition and amorphization due to surface impurities," Nanoscale 8(23), 11803-11809 (2016). (doi:10.1039/C5NR09027J) 12.2.2

(12) Luz, Ignacio, Anna Loiudice, Daniel T. Sun, Wendy L. Queen, and Raffaella Buonsanti, "Understanding the Formation Mechanism of Metal Nanocrystal@MOF-74 Hybrids,"Chemistry of Materials 28(11), 3839-3849 (2016). (doi:10.1021/acs.chemmater.6b00880)12.2.2

(13) Mao, H.K., B. Chen, J. Chen, K. Li, J.-F. Lin, W. Yang, and H. Zheng, "Recent advances in high-pressure science and technology," Matter and Radiation at Extremes 1(1), 59-75 (2016). (doi:10.1016/j.mre.2016.01.005) 12.2.2,12.3.2

(14) Miller, Reece G., Suresh Narayanaswamy, Simon M. Clark, P.K. Dera, Geoffrey Jameson, Jeffery Tallon, and Sally Brooker, "Pressure induced separation of phase-transition-triggered-abrupt vs. gradual components of spin crossover," Dalton Transactions 44(48), 20843-2084 (2015). (doi:10.1039/C5DT03795F) 12.2.2

(15) Miyagi, L., and H.-R. Wenk, "Texture development and slip systems in bridgmanite and bridgmanite + ferropericlase aggregates," Physics and Chemistry of Minerals 43(8), 597-613 (2016). (doi:10.1007/s00269-016-0820-y) 12.2.2

(16) O'Bannon, Earl, and Quentin Williams, "Beryl-II, a high-pressure phase of beryl: Raman and luminescence spectroscopy to 16.4 GPa," Physics and Chemistry of Minerals 43(9), 671-687 (2016). (doi:10.1007/s00269-016-0837-2) 12.2.2

(17) Palaich, Sarah.E.M., "Carbon in the Deep Earth: A Mineral Physics Perspective," doctoral dissertation, University of California, Los Angeles, Los Angeles, CA, USA, 2016, advisor Abby Kavner. 12.2.2

(18) Palaich, S.E., R. Heffern, A. Watenphul, J. Knight, and A. Kavner, "High-pressure compressibility and phase stability of Mn-dolomite (kutnohorite)," American Mineralogist 100(10), 2242-2245 (2015). (doi:10.2138/am-2015-5095) 12.2.2

(19) Raju, S.V., B.K. Godwal, J. Yan, R. Jeanloz, and S.K. Saxena, "Yield strength of Ni–Al–Cr superalloy under pressure," Journal of Alloys and Compounds 657, 889-892 (2 2016). (doi:10.1016/j.jallcom.2015.10.092) 12.2.2

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Appendix 2. Beamline Schedules

Nov-15	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	Sa	Su	M
0000-0800																										H	H	X	X	
0800-1600													Maintenance Shutdown													H	H	X	X	
1600-2400																										H	H	X	X	

Dec-15	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th
0000-0800																								H	H	X	X	H	H	H	H
0800-1600							Maintenance Shutdown									Maintenance Start-Up & Tune								H	H	X	X	H	H	H	H
1600-2400																							X	H	H	X	X	H	H	H	H

JANUARY IS PART OF CYCLE

Jan-16	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su
0000-0800	H	X	X	IT														H	IT	I	s.o.					MS					
0800-1600	H	X	X	Maintenance Start-Up & Tune				BL C			BLC		m/c	DD	IHR	McCluskey		H	M	I	JY	Santamaria-Perez 7565			AP	Jeanloz		Chen-Hawaii			
1600-2400	H	X	X													6875		H	I	S/T	734				AP	6741		6556			

ALS beamline 12.2.2 operation schedule

January - June 2016

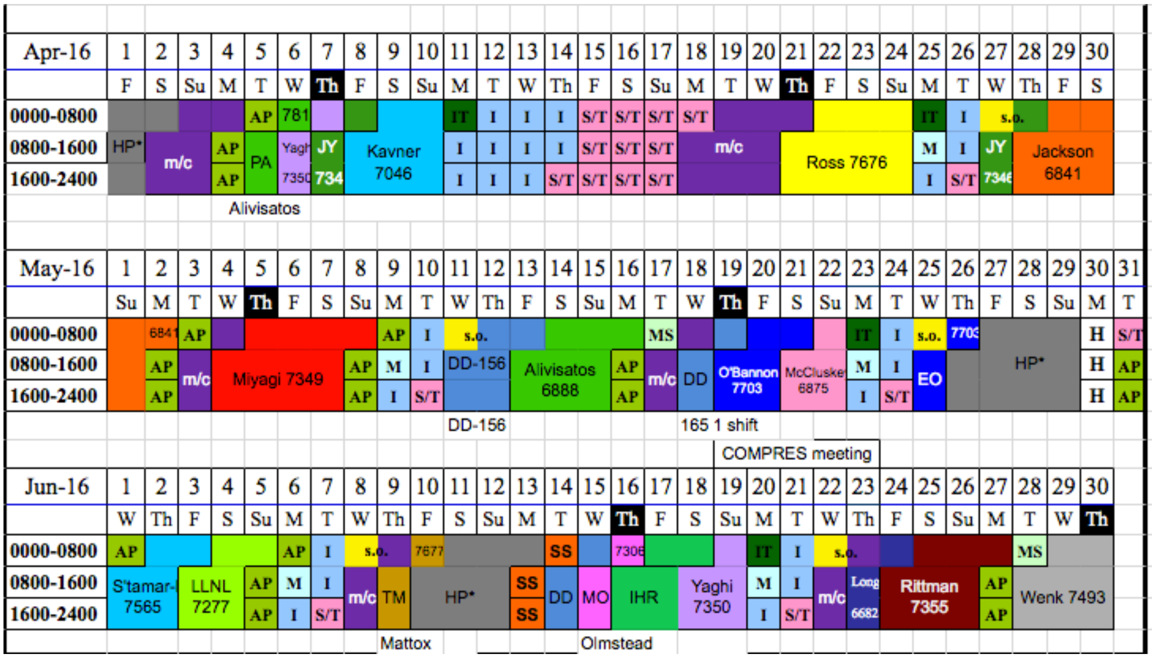
COMPRES

JANUARY IS IN CYCLE 2015-2 - ONLY SHOWN FOR CONVENIENCE

Jan-16	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	Tu	W	Th	F	S	Su	M	T	W	Th	F	S	Su
0000-0800	H	X	X	IT	S/T	S/T	S/T	S/T	S/T	S/T	S/T	BLC	BLC					H	IT	I	s.o.					MS					
0800-1600	H	X	X	S/T	S/T	S/T	S/T	BLC	S/T	S/T	BLC	BLC	m/c	DD	IHR	McClusk		H	M	I	JY	Santamaria-			AP	Jeanloz		Chen-Hawaii			
1600-2400	H	X	X	S/T	S/T	S/T	S/T	S/T	S/T	S/T	BLC	BLC				6875		H	I	S/T	734	7565			AP	6741		6556			

Feb-16	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29
	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M
0000-0800		I	s.o.						AP						H	IT	I	s.o.					MS						MS
0800-1600	M	I	Long	Yagh	Ciezak 7309			AP	DD	m/c		McCluskey 6875			H	M	I	JY	Chan 7881			AP	m/c	IHR		Monteiro 7680		AP	M
1600-2400	I	S/T	6682	7350				AP							H	I	S/T	7340				AP						AP	I
									162																				

Mar-16	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th
0000-0800	I	s.o.					AP							IT	I	AP	s.o.						MS						I	s.o.	
0800-1600	I		Gilbert 7964			AP	m/c		DD	IHR		Tolbert 6767		M	I	AP			2-bunch			AP			2-bunch			M	I	HP*	
1600-2400	S/T					AP								I	S/T	AP						AP						I	S/T		
									165																						


Apr-16
0000-0800
0800-1600
1600-2400
HP*
m/c
AP
PA
Yagh 7350
781
JY 734
Kavner 7046
IT
I
S/T
M
m/c
Ross 7676
s.o.
JY 7346
Jackson 6841
Alivisatos
May-16
6841
Miyagi 7349
DD-156
Alivisatos 6888
MS
DD
O'Bannon 7703
McCluskey 6875
EO
7703
HP*
H
DD-156
165 1 shift
COMPRES meeting
Jun-16
S'tamar 7565
LLNL 7277
TM
7677
HP*
SS
DD
MO
7306
IHR
Yaghi 7350
Long 6682
Rittman 7355
Wenk 7493
Mattox
Olmstead

ALS beamline 12.2.2 operating schedule

July - December 2016

Jul-16	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	Tu	W	Th	F	S	Su	M	T	W	Th	F	S	Su
0000-0800	Wenl			H	IT	M/I	s.o.					AP						IT	M/I	s.o.						AP					
0800-1600	Tolbert 8381			H	M/I	M/I	DD	Ciezak-J 7909			AP	JY	m/c	IHR		OT 8146		M/I	M/I	Long	IHR	Santamaria-Pe rez 7565			AP	m/c			Liu 7386		AP
1600-2400				H	M/I	S/T					AP	7346						M/I	S/T	8376					AP						AP
							DD-195																								

Aug-16	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W
0000-0800	AP	M/I	s.o.					AP	7376						IT	M/I	AP							AP					IT	M/I	s.o.
0800-1600	M/I	M/I	m/c	DD			AP	Alivisatos		IHR		HP* AP			M/I	M/I	AP	2-bunch					AP		2-bunch				M/I	M/I	m/c
1600-2400	M/I	S/T					AP								M/I	S/T	AP						AP						M/I	S/T	

Sep-16	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F
0000-0800					H	S/T	AP	7493	7814			IT	M/I	s.o.						AP			7680			AP	M/I	s.o.	7306	
0800-1600	m/c	JY	Yaghi 7350		H	AP	Wen	Ali visa tos	McCluskey 6875			M/I	M/I	DD	m/c	Stavrou 8127			AP	QW / EO'B 7703		Mo ntei ro	Alivisato s 7869		AP	M/I	M/I	Ol mst ead	Gur lo AP	7802
1600-2400		7346			H	AP						M/I	S/T						AP						AP	M/I	S/T			

			Users Meeting																												
Oct-16	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M
0000-0800			IT	M/I	M/I	M/I	S/T	IT	IT	s.o.							AP							AP	M/I	s.o.					
0800-1600	Zeng 7802		M/I	M/I	M/I	M/I	IT	IT	IT	m/c	Gur lo AP	Gilbert 7964		JY	Gur lo AP	AP	m/c		EOB	HP* AP			AP	M/I	M/I	Zeng 7839			Gurlo AP		AP
1600-2400			M/I	M/I	M/I	S/T	IT	IT	IT					7346		AP							AP	M/I	S/T						AP

Nov-16	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W
0000-0800	AP		7493				IT	M/I	s.o.						AP						AP			H	H	H	H	IT	M/I	s.o.
0800-1600	Gur lo AP	Wen		Miyagi 7349			M/I	M/I	Shim 8225		Kavner 7046			AP	Long		Jackson 6841			AP	Long	Jacob 7931		H	H	H	H	M/I	M/I	
1600-2400							M/I	S/T						AP	8376					AP	8376			H	H	H	H	M/I	S/T	

Dec-16	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S	Su	M	T	W	Th	F	S
0000-0800	Sta vro u 727 7					AP	7493					AP	M/I	s.o.	7677							AP	H	H	H	H	H	H	H	H	H
0800-1600		QY/Cara 8337			AP		Wen		HP* AP		AP	M/I	M/I	Mat tox	DD	IHR	Turner 7698		IHR	Monteiro 7680		AP	H	H	H	H	H	H	H	H	H
1600-2400					AP						AP	M/I	S/T									AP	H	H	H	H	H	H	H	H	H