ALS Beamline 12.2.2

2015 COMPRES Annual Report

November 2014 – October 2015

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Overview

- Last year's publications, and this year's
    - High percentage of high profile papers
    - User office truck up
- Staffing changes-status
    - AD Settling in, MK is supervisor
    - HPSTAR postdoc
    - ALS Doctoral Fellow

The history of beamline 12.2.2 is littered with dramatic tales of ruin and rebirth. After the painful circumstances of the ALS reduction in force in 2014 (which resulted in the losses of Jason Knight and Bora Kalkan), 2015 has been refreshingly positive, with great strides taken in experimental facilities, user satisfaction, and in the latter half of the year, requests for beamtime. The reconfigured beamline staff, ALS and COMPRES together, have become a cohesive team under the leadership of Martin Kunz and Quentin Williams, with advisory support given by Alastair MacDowell.

The new, completely redesigned laser heating system has received glowing reviews in its first year as a user facility. The new design has performed impressively in all aspects: operation and temperature determination are straightforward and heating levels of samples is now purely sample dependent, unlike in the previous design. Indeed, prior issues of mechanical stability have been entirely removed, with the new compact and mechanically robust design; and the optics themselves have been improved. As an important ancillary note, this redesign and rebuild was entirely funded by the ALS facility. Axial laser heating is now considered a routine user request, and the ruggedness of the system has allowed Kunz and COMPRES' Jinyuan Yan to focus their energy on further expansion of the laser heating facility to incorporate radial methods, which will emerge from commissioning in the new year. In addition, the laser heating pyrometry software will also soon include 2-D hot spot profiling, coded by Yan. These innovations will ensure that 12.2.2's position as a world class laser heating facility is secure.

The COMPRES mandate for high-pressure single crystal capabilities has been a powerful force on 12.2.2. It inspired the hiring of Christine Beavers, which has enabled the current single crystal system. Although heavily improvised, this system has enabled the collection of quality high pressure single crystal data for approximately 15 groups over the last two years. The weaknesses of this system are numerous, however, and the goal has always been to acquire better diffractometry to enable high quality single crystal work. In September of this year, ALS management allocated funds for the purchase of **both** a 4-circle diffractometer and a CMOS fast detector. This is a major investment by the ALS facility in high-pressure single crystal capabilities at the ALS, and continues the extremely large leveraging of facility-derived money by the COMPRES effort. These purchases, when finalized, will create a dedicated high pressure single crystal facility, with specifications unmatched by any other beamline in the world. The project management and engineering skills of Andrew Doran (who was assigned to 12.2.2 by the facility after the departure of Knight) are being fully employed towards the successful completion of this project, which is being overseen by Beavers and Kunz. The installation of the system is planned for early 2016, with commissioning tentatively planned for spring 2016.

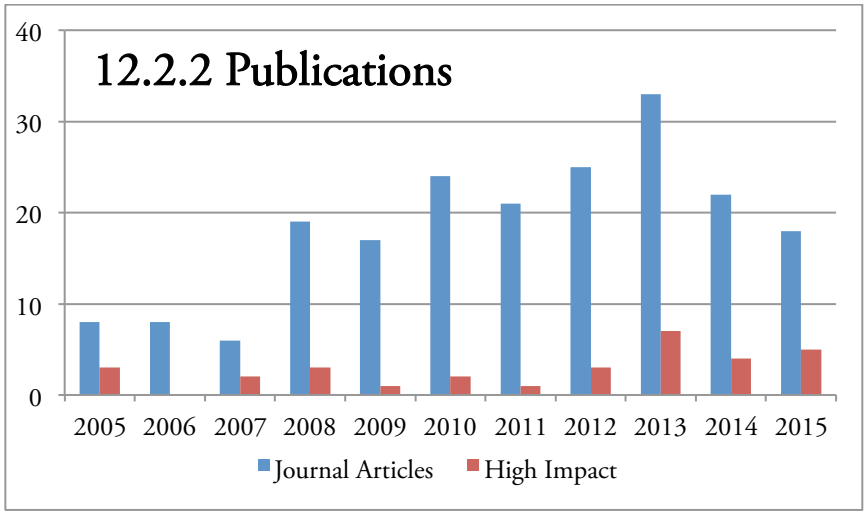
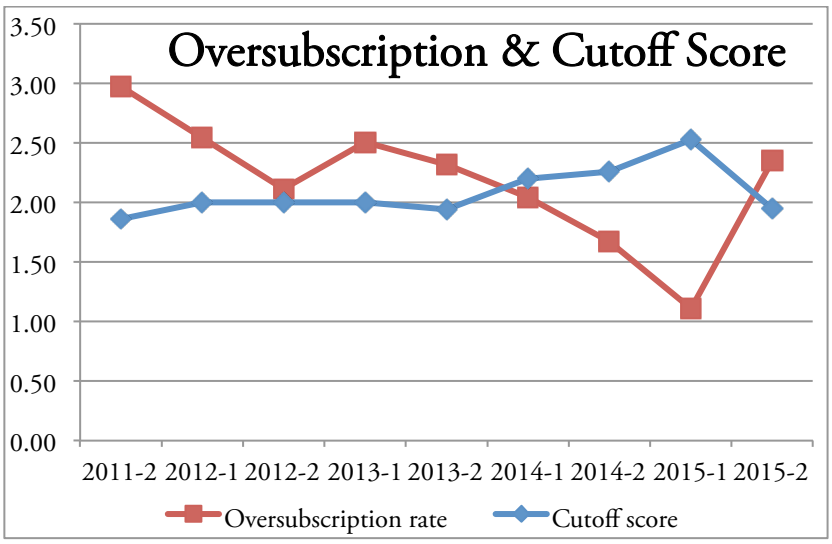


Figure 1. Publication trends through time at 12.2.2, as recorded in the ALS publication database. Numbers for 2015 are through 10/20/15, and hence reflect both an incomplete year and the usual lags of PIs posting their publications.

Beamline performance, as measured by the traditional metrics, has been respectable, and is showing signs of a substantial shift in proposal competitiveness. As shown in the above chart, publications have taken a dip since the banner year of 2013, but the current level of production is within the normal range, considering the difficult experiments done on 12.2.2. Recent years have also shown an increase in the percent of publications in "DOE High impact" journals; this increase could relate to the lower overall publication numbers, since high impact work is generally more difficult and time consuming.



Other metrics that can be analyzed are the oversubscription rate and the cutoff score for proposals allocated. These can indicate the user community demand and the quality of proposals allocated, respectively. The oversubscription rate had been gradually falling since 2013, but has now rebounded sharply, which also drove the cutoff score lower. The notable downturn in 2015-1 was clearly associated with a change in how the user office notified users about their renewals: this is described in the Beamline Operations section below—this was clearly an aberration. Notably, the recent change in 2014-2 towards greater oversubscriptions does not appear to be a fluke--the allocations for 2016 have not yet been done, but the requests for time are more impressive than they were in 2015-2, and this is also discussed further below. These metrics indicate what we on the beamline can gauge from users in person: beamline 12.2.2's standing in the user community has been improved, primarily because of the current staff's dedication to improving the user experience and the experimental facilities.

Scientific Highlights

To emphasize our facility's continued dedication to state-of-the-art radial diffraction, we present the following highlight, entitled "Slab stagnation in the shallow lower mantle linked to an increase in mantle viscosity" from Marquardt and Miyagi (Nature Geosci., 8, 311–314, **2015,** Figure 2 shown below.). Their careful examination of the deformation behavior of (Mg,Fe)O ferropericlase, using radial diffraction on beamline 12.2.2, indicates that a substantial viscosity increase in this material may be responsible for the slab stagnation within the shallow lower mantle that has been observed in a range of subduction zones with seismic imaging. Specifically, in high strain regions where ferropericlase is anticipated to be interconnected, the substantial increase in strength (and hence viscosity) is anticipated to impede slab penetration; at deeper depths, weakening associated with the spin transition of iron may generate a viscosity structure that is peaked in the shallow lower mantle. Previous studies to examine this behavior had not employed radial, angle dispersive techniques, and therefore had been blind to the texture and strain development.

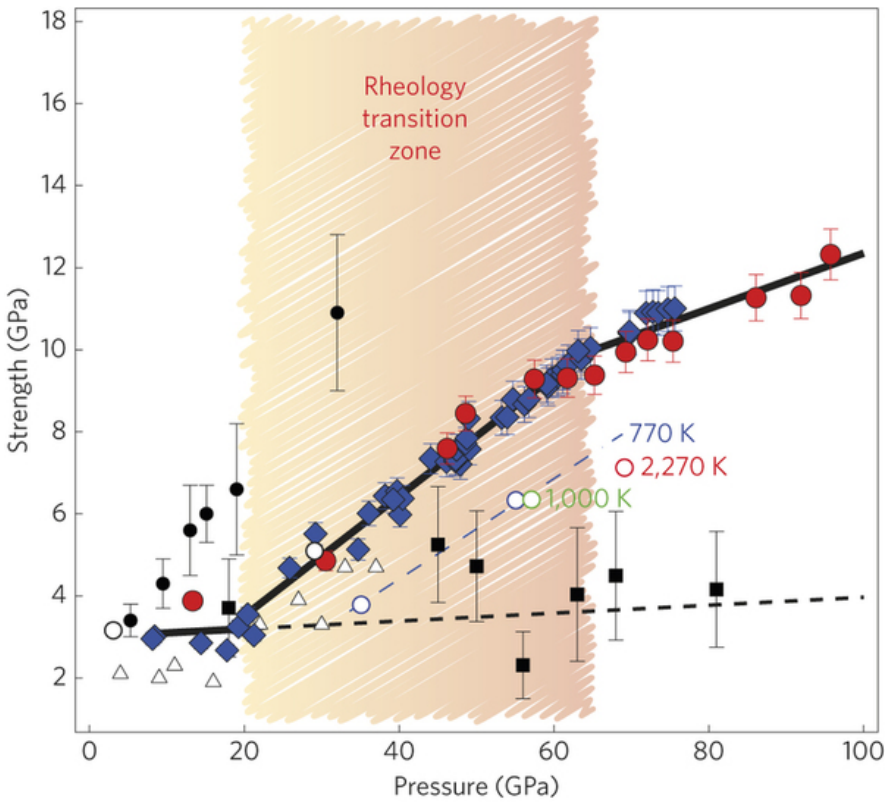


Figure 2: Red circles & blue diamonds, new measurements from Marquardt and Miyagi (2015) at 12.2.2. Solid black lines, linear fits to data in the pressure ranges <20 GPa, 20–65 GPa and >65 GPa. Dashed black line, linear extrapolation of data at pressures <20 GPa. Black squares, $(Mg_{0.83}Fe_{0.17})O$ (Lin et al., PCM, 2009), White triangles, $(Mg_{0.4}Fe_{0.6})O$ (Tommaseo et al., PCM, 2006). White circles, blue dashed line, $(Mg_{0.8}Fe_{0.2})O$ (Miyagi et al., RSI, 2013). Black circles, $(Mg_{0.9}Fe_{0.1})SiO_3$ bridgmanite (Merkel et al., EPSL, 2003).

Our second highlight comes from the materials science community (with the engagement of a COMPRES collaborator), where there has been a growing interest in the capabilities of 12.2.2, and focuses on a crystal structure of considerable importance within the high-pressure geosciences. Organic-inorganic perovskites are a burgeoning area of interest in materials science, due to their magnetic, luminescent and conduction properties. In this highlight, from A. Jaffe, Y. Lin, W.L. Mao and H.I. Karunadasa (J. Am. Chem. Soc., 137(4), 1673-1678, **2015,** Figure 3 shown below), two-dimensional Cu-Cl hybrid perovskites were subjected to pressure, in order to monitor the evolution of their structural and electronic properties. The authors were able to observe two phase changes, and determine the bulk moduli, using 12.2.2 PXRD, as well as measure the appearance of

semiconductor behavior under pressure.

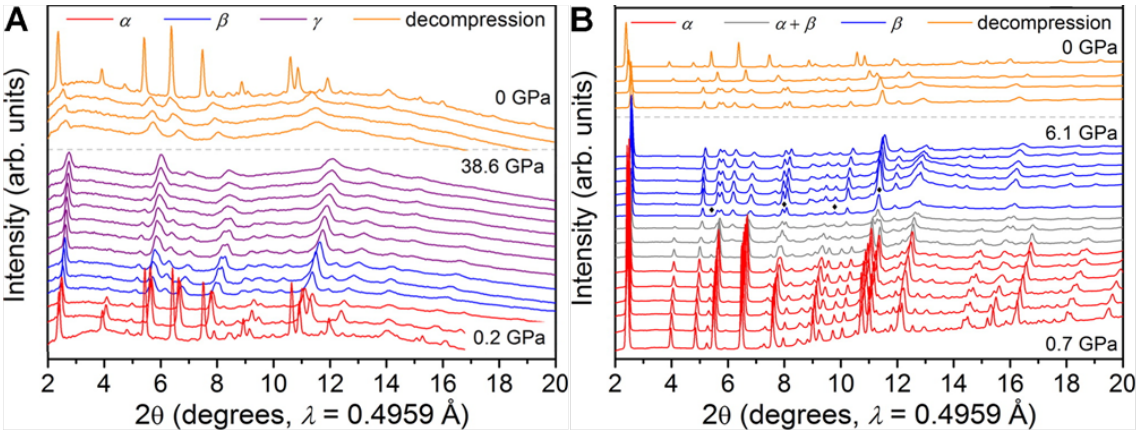
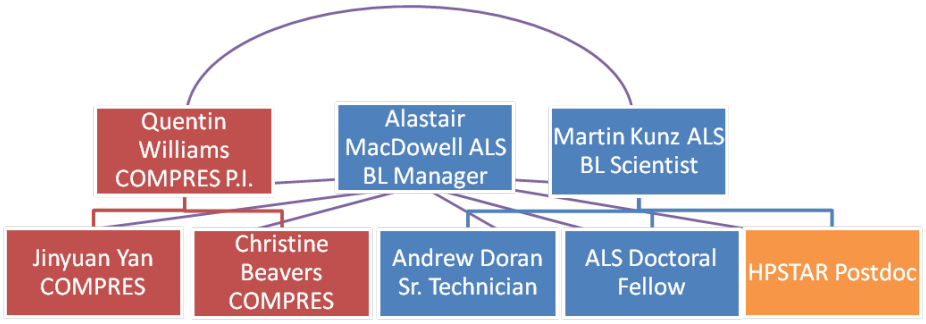


Figure 3: (A) PXRD patterns of **(ethylenedioxy)bis(ethylammonium)[$CuCl_4$] (known as (EDBE)$CuCl_4$)** upon compression up to 38.6 GPa and decompression to ambient pressure. Data acquired above ca. 8 GPa are shown in purple because EOS fitting indicated a third phase (γ). (B) High-resolution PXRD patterns for **(EDBE)$CuCl_4$** during compression to 6.1 GPa and decompression to ambient pressure.

The high profile aspect of this article isn't so much the outcomes of the high pressure experiment, but the fact that high pressure is being used as a tool for structural perturbation of a complex, technologically interesting material. This is becoming more attractive to the materials science community, which is giving rise to tougher competitions for beamtime. In terms of future work from this group, they are currently finalizing single crystal HP studies on other materials of this type from work at 12.2.2, and submission of a publication on these results is imminent.

Beamline Personnel



The core personnel responsible for beamline 12.2.2 has not changed a great deal in the last year, as shown in the above organizational chart (red and blue lines indicate supervisory roles, purple lines indicate advisory roles). MacDowell has ceded most supervisory responsibilities to Kunz, and

remains involved in an advisory role. Doran now answers directly to Kunz as his line manager. On the COMPRES side, Beavers and Yan continue to develop their respective projects and support the COMPRES community, which is detailed in their individual annual reports. The most notable staffing developments concern the recent additions of 2 consecutive ALS doctoral fellows, and the stationing of 2 HPSTAR post-docs, one of which is specifically dedicated to 12.2.2.

ALS doctoral fellows are awarded on a competitive basis, and are not directed at a particular beamline outside of the desired work of the applicant. In 2015, Anya Rasmussen, a student of Matt McCluskey at Washington State University, completed her year on 12.2.2. Her research focus was on HP PXRD at modestly high temperatures on semiconductor materials (300-900°C); her technical focus was the implementation of a ceramic ring heater for the BX90 DAC. By the end of her tenure, Rasmussen had successfully collected data at the desired temperatures and the ring heater was shown to be a readily accessible avenue to achieve modest temperatures. The incoming ALS fellow on 12.2.2, Earl O'Bannon, a student with Quentin Williams at UC Santa Cruz (who has already spent considerable time at 12.2.2), plans on modifying the ring heater for use in single crystal work, in order to study the behavior of subduction zone minerals at high pressures and temperatures. This development will be synergistically amplified by the new single crystal diffractometer, with which he will be engaged. Through the funding of these two fellows, the ALS has sponsored the testing and commissioning of a new user facility which will predominantly benefit the mineral physics community. COMPRES PIs are urged to consider ALS doctoral fellowships for synchrotron-minded students in the future (application deadlines are June 30).

The Approved Program (AP) proposal submitted by HPSTAR included the promise of two post-docs stationed at the ALS, one for 12.2.2, and one for the Laue microdiffraction beamline 12.3.2. This promise was mostly unfulfilled until this fall, with the arrival of Binbin Yue and Fang Hong, who will be working primarily on 12.3.2 and 12.2.2 respectively. Both have DAC experience and both are interested in radial diffraction as well as single crystal diffraction. We are optimistic that they will be an asset to the beamline community.

Continued COMPRES support for beamline 12.2.2 is seen by ALS management as robust, and in that light, they are more willing to match this support with ALS staff and capital equipment monies. For this year, ALS management has nearly matched the COMPRES 12.2.2 commitments with 12.2.2 *equipment purchases alone* (note that we are not including the ALS salary commitments to Kunz and Doran, which would make ALS' contribution this year **far** exceed those of COMPRES to the staffing and development of instrumentation at the beamline). A pertinent quote on this is taken from last year's report:

"For reference, were COMPRES support discontinued (for whatever reason), the high-pressure/geosciences emphasis of 12.2.2 would be re-evaluated, and it would be fully anticipated that the ALS staff commitment would be redeployed away from geosciences-oriented projects (both materials science

and environmental science-related applications could be notably enhanced at 12.2.2 in such a scenario). In this context, the COMPRES effort leverages a VERY large staff salary match from the ALS for the high-pressure enterprise at LBNL."

The organization of the beamline staff predominately occurs during weekly meetings, now usually on Monday afternoons. In these work planning meetings, maintenance tasks and upgrade projects are discussed and prioritized. User needs for the upcoming week are also clarified, as well as any questions on support. Every staff member is asked to give feedback on their progress on existing projects. This meeting provides a valuable channel for all staff to communicate freely, and has created a more cohesive team.

ALS/12.2.2 Approved programs

The COMPRES Approved Program was renewed for the term of Jan 2015- Dec 2018. The new proposal, from COMPRES President Bass, requested an increase of guaranteed time on beamline 12.2.2, from 35% to 50%, but this increase was declined by the ALS science director: this declination may have been generated (partially or wholly) by the COMPRES community's recognized success in getting time at 12.2.2 well in excess of 35% through the General User Program.

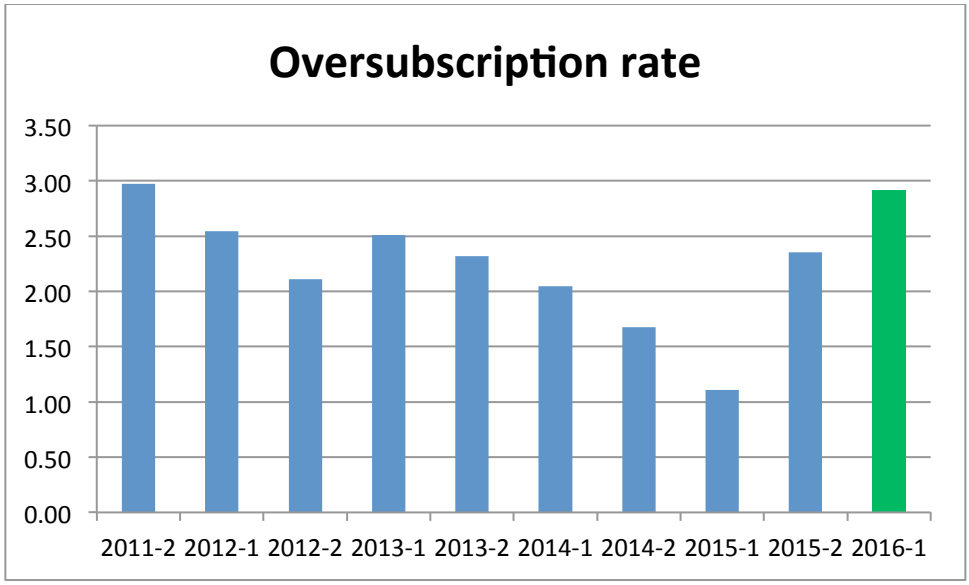
The HPSTAR AP, originally allocated 10% of the time at 12.2.2, has been under some duress to produce some of the promised manpower and equipment. Their allocations were reduced to 5% of the available shifts in 2015-2, to induce some compliance with the memorandum of understanding. To this end, the reductions were successful- two post-docs were hired, a new microscope has been bought, and a micromanipulator is being actively researched for purchase. No other APs have been proposed for beamline 12.2.2.

Beamline Operations

In the last year, beamline operations have been fairly continuous and smooth. There have been no major maintenance outages during the reporting period of Nov 2014- Oct 2015, but a major installation and upgrade to the synchrotron RF system is precipitating an outage from Nov 2015-Jan 2016—fortunately, as with some past maintenance outages, this spans over the winter holidays, and hence is anticipated to have a lesser effect on users' perceptions or research programs than mid-year outages.

The chart below illustrates the oversubscription rate of beamline 12.2.2 (requested shifts/allocated shifts). Historically, the oversubscription rate on 12.2.2 has been consistently above 1.5 (66% of requests allocated), so we were rightfully confused when requests in 2015-1 were much lower than previous years. This was soon recognized as being associated with a major change in how

the ALS User office was interacting with users; proposal PIs, who had always been sent personalized email reminders to resubmit their proposals, were now only receiving one generic "call for proposals" email. This change had a surprisingly large impact, and beamline scientists were not informed in advance of the change—its impact was not recognized until proposals were submitted. Numerous other beamlines at the ALS suffered the same drop, for the same reason.



The second allocation period of 2015 was much more successful, with a return to a far more favorable oversubscription rate. We credit this to vigilant reminding of PIs coupled with community outreach about our improved facilities for laser heating and single crystal. The first allocation period of 2016 looks to be even more competitive; allocations have not yet been done, but requests have surpassed those of 2015-2, and a similar number of available shifts is expected. The new challenge will be to continue to keep applying users engaged- high oversubscription rates usually falter when repeat applicants become disillusioned after multiple rejected proposals. Maintaining momentum may require allocating small amounts of beamtime (1 day) to lower rated proposals, to whet their appetite and maintain their interest in the facility.

Our beamtime allocations and schedules are given in Appendices 2 and 3. The numerical description of General User allocations is:

196 8-hour shifts available and 328 requested in July-Dec., 2014 (59.8% available/requested, 1.67:1 oversubscription rate---23 proposals given time, 37 proposals total).

225 8-hour shifts available and 249 requested in Jan-Jun., 2015 (90.4% available/requested, 1.11:1 oversubscription rate---25 proposals given time, 29 proposals total).

196 8-hour shifts available and 461 requested in July-Jan., 2015 (42.5% available/requested, 2.35:1 oversubscription rate---23 proposals given time, 53 proposals total). This is a seven month allocation period to compensate for a lengthy upgrade shutdown (Nov-early Jan).

In the template for this report, COMPRES has requested statistics for the past two years. Below are the data on allocations in the 2013(1 & 2) and 2014-1 allocation periods.

204 8-hour shifts available and 539 requested in Jan-July 2013 (39.9% available/requested, 2.51:1 oversubscription rate---21 proposals given time, 47 proposals total). This was a seven month allocation period to compensate for a lengthy upgrade shutdown.

204 8-hour shifts available and 473 requested in Aug-Dec 2013 (43.1% available/requested, 2.32:1 oversubscription rate---21 proposals given time, 50 proposals total). This was a five month allocation period to compensate for the previous allocation period extension.

215 8-hour shifts available and 440 requested in Jan-June 2014 (48.9% available/requested, 2.05:1 oversubscription rate---25 proposals given time, 45 proposals total).

Performance Metrics

In the Nov 2014- Oct 2015 span, we had 30 distinct research groups visit the ALS to use 12.2.2. Of these, 25 were affiliated with universities, three with national labs, and two with a foreign, private foundation (HPSTAR). Among all groups, only three were foreign: two HPSTAR groups and a group from Tel Aviv University, Israel. The funding sources and days allocated for these groups are listed in the performance metrics section.

Our estimate for the 2014-2015 year is that we had ~68 users, with 54 from universities, and the balance from labs. Of these 68, 31 were graduate students. The unique users include 32 with COMPRES affiliations, with 21 of these being graduate students. We did not record any undergraduate users in the past year.

COMPRES users made up 51.5% of allocated shifts over the course of Nov 2013-Oct 2014. In this reporting year, the percentage of shifts allocated to COMPRES users is 50.4%. In both cases, 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	2014-2	11/1/14-12/31/14											
PI Name	# days	Beam time	COMPRES User ©	Funding Source	Country	NSF-EAR	NSF-DMR	NSF-Chem	DOE	DOD	NSF-China	NNSA	Foreign
Bhat	3	11/11-11/14		NNSA/DOE	USA				1			1	
Bin Chen(HP*)	6	11/7-11/10; 12/9-12/11; 12/17-12/18		Foreign (NSF)	China						1		1
Deemyad	1.66	8/29-8/30		NSF-DMR	USA		1						
Godwal	4	11/20-11/22;11/24-11/26	C	DOE	USA				1				
Kaner	2	11/14-11/16	C	NSF-Chem	USA			1					
Karundasa	2	11/6-11/7; 12/4-12/5		NSF-Chem	USA			1					
McCluskey	1.33	11/16,11/18-11/19		NSF-DMR	USA		1						
Miyagi	3.66	12/11-12/14	C	NSF-EAR	USA	1							
Tolbert	2.66	12/5-12/8	C	NSF-DMR	USA		1						
Willams	4	11/5-11/6; 12/19-12/22	C	NSF-EAR	USA	1							
Yang	2	11/22-11/24		NSF-DMR	USA		1						
			45.45%										
	2015-1	1/1/15-6/30/15											
PI Name	# days	Beam Time											
Alivisatos	4	2/5-2/9		DOE-MSE	USA				1				
Bin Chen (HP*)	11	2/12-2/15;3/26-3/29; 6/11-6/14		Foreign (NSF)	China						1		1
Bin Chen(Hi)	2	4/24-4/26	C	NSF-EAR	USA	1							
Ciezak-Jenkins	5	2/27-3/1; 5/1-5/4		DOD	USA					1			
Deemyad	3	5/8-5/11		NSF-DMR	USA		1						
Forster	3	2/20-2/23		DOE	USA				1				
Godwal	7.33	3/12-3/15; 5/21-5/24	C	DOE	USA				1				
Jackson	5.66	5/12-5/17	C	NSF-EAR	USA	1							
Jeanloz	3.66	1/15-1/18	C	DOE	USA				1				
Karundasa	4	1/29-1/30;3/20-3/21;4/30-5/1;6/7-6/8		NSF-Chem	USA			1					
Kavner	2	1/30-2/1	C	NSF-EAR	USA	1							
Levy	2	6/9-6/11		Foreign (NSF)	Israel								1
Long	2	3/21-3/22; 3/29-3/30		NSF-Chem	USA			1					
McCluskey	3.66	1/25-1/26;3/22-3/23;5/32;6/29-6/30		NSF-DMR	USA		1						
Mi	2	2/10-2/12		Foreign (NSF)	China						1		1
Miyagi	4	6/18-6/22	C	NSF-EAR	USA	1							
Ross	2	3/24-3/26	C	NSF-EAR	USA	1							
Sun	1	6/30-7/1		NSF-DMR	USA		1						
Tolbert	3	3/6-3/9	C	NSF-DMR	USA		1						
W. Mao	4	1/23-1/25;4/17-4/19	C	NSF-EAR	USA	1							
Williams	10	2/4-2/5; 3/5-3/6; 4/21-4/24; 5/27-5/28; 5/5-5/7; 5/26-5/28	C	NSF-EAR	USA	1							
			50.00%										
ALS 12.2.2	2015-2	7/1/2015-11/1/2015											
PI Name	# days	Beam Time											
Alivisatos	3	8/27-8/30		DOE-MSE	USA				1				
Bin Chen(Hi)	2	9/19-9/21	C	NSF-EAR	USA	1							
Bin Chen(HP*)	4.33	9/9-9/13		Foreign (NSF)	China						1		1
Ciezak-Jenkins	3	10/9-10/12		DOD	USA					1			
Clearfield	1	10/17-10/18		NSF-Chem	USA			1					
Jackson	3	10/2-10/5	C	NSF-EAR	USA	1							
Karundasa	2.33	7/23-7/24; 8/20-8/21; 9/22-9/23		NSF-Chem	USA			1					
Kavner	3	7/24-7/27	C	NSF-EAR	USA	1							
Long	2	8/1-8/2; 10/20-10/21		NSF-Chem	USA			1					
McCluskey	2.66	9/17-9/18; 9/26-9/27		NSF-DMR	USA		1						
Mi	2	7/11-7/13		Foreign (NSF)	China						1		1
Miyagi	4	8/21-8/26	C	NSF-EAR	USA	1							
Olmstead	2	8/1,8/2; 8/19-8/20		NSF-Chem	USA			1					
Ross	2	10/14-10/16	C	NSF-EAR	USA	1							
Stavrou	5	9/23-9/25; 10/16-10/19		NNSA/DOE	USA				1			1	
Tolbert	2.66	9/18-9/21	C	NSF-DMR	USA		1						
Tschauner	2	7/28-7/29; 10/8-10/9	C	NNSA/DOE	USA				1			1	
W.Mao	2	10/21-10/23	C	NSF-EAR	USA	1							
Wenk	3	10/23-10/26	C	NSF-EAR	USA								
Willams	5	7/15-7/16; 7/17-7/18; 7/30-7/31; 9/3-9/4; 10/1-10/2;	C	NSF-EAR	USA	1							
Yaghi	3	7/1-7/2; 7/18-7/19		DOE	USA								
			47.62%	Totals	40	14	7	6	7	2	4	2	6
*NNSA supported users were all also DOE supported						28.57%	14.29%	12.24%	14.29%	4.08%	8.16%	4.08%	15.00%
All time was allocated through the GU panel, with the exception of the HPSTAR Approved program, which received 10% of available time in 2014-2 and 2015-1, and 5% of time in 2015-2.						NSF-EAR	NSF-DMR	NSF-Chem	DOE	DOD	NSF-China	NNSA*	Foreign

Beamline Development/Planned Activities

This year's development activities have been focused on commissioning the radial laser heating, and preparing for the renovation of End-Station 1 (ES1) to include the new single crystal diffractometer. The radial laser heating commissioning has been assisted by Lowell Miyagi (U. Utah), who has been invaluable in analyzing and understanding the technical difficulties that have arisen. The radial laser heating system is nearly ready to become a user facility.

The single crystal program received a sizable boost when ALS funds were allocated to purchase a Stoe Stadi-Vari 4-circle diffractometer with an Eulerian cradle and a CMOS fast detector from RDI. This disbursement of ~$250k has put the high pressure single crystal program on track for a potential spring 2016 installation, with commissioning to follow. At this time, conceptual work for implementing the ordered system is coming to a conclusion, with two heavy duty stages, a motorized collimator and some minor endstation remodeling required. To expedite the installation, and involve the COMPRES enterprise, we are submitting a proposal to the COMPRES EOIC call to fund the stages and the collimator.

Beamline Community Activities

The COMPRES staff members have described their activities under a separate request for input from them, and COMPRES is referred to the 12.2.2 beamline scientists' reports for more information. Beavers has engaged in considerable community outreach at the American Crystallographic Association annual meeting, from distributing beamline information at the ALS sponsored booth, to giving a lecture describing the capabilities of 12.2.2, while also guiding next year's program to include sessions with a mineral physics theme. With the upcoming installation of the single crystal system, we have deferred our previous plan to do a high P/T single crystal workshop until the new system is ready, potentially coinciding with the ALS user meeting 2016. We have also considered joining forces with beamline 11.3.1 (which has very substantial single-crystal diffraction expertise, including at extreme conditions) to hold a single crystal master class for experienced crystallographers, to introduce in-situ experiments.

Budget Justification for Next Cycle:

Personnel: Beavers and Yan both were reclassified this past year: Beavers to Assistant Researcher Step V, and Yan to Project Scientist Step III. UC has given 3% cost of living augmentations the last three years. Fringe benefits on both positions are requested. As part of a COMPRES Ex Comm approved match to an ALS Doctoral Fellow award to Earl O'Bannon, 4 months @ $750/month of GSR funding (June-September) is also requested.

Supplies and Expendables: Funding is requested for expendables utilized by users at the beamline. This includes items such as replacement parts for equipment utilized by users, such as custom DAC rigs for the gas-loading apparatus, replacement parts for the laser miller (which we hope to move off

the books during the coming year with a new recharge system—we do not anticipate that this will impact COMPRES users), sample preparation equipment, our ruby fluorescence apparatuses, gasket materials, locally-made external heaters, and other materials that just seem to be used up by users.

Travel: A budget for travel is requested. This will be utilized primarily for the beamline scientists to attend meetings (including the COMPRES meeting: these are important for their professional development, their knowledge of new techniques, and for acquiring new potential users of the beamline) and to occasionally visit other major facilities to share best practices and to exchange expertise. An additional $2500 in international travel is requested to allow Beavers to attend the European Crystallographic meeting in 2016, which has a large number of mineral physics and high pressure oriented sessions. This exposure would be helpful when considering the current state of the art of high pressure single crystal, and allow contact with the current European state-of-the-art in this domain.

Equipment: An EOID proposal for equipment pertaining to the single crystal system has been submitted separately.

Beamline Support from the Facility: The ALS provides 2 FTE in staff support, as well as a large amount of capital equipment money. In addition to the funding this year for the diffractometer and detector, the ALS funded the gas loading system and the complete renovation of the laser heating system and many smaller necessary components, i.e., diamonds, DACs, etc. The ALS provides funds for 12.2.2 upkeep and consumables, which totals ~$60k per year. Thus, in the last year, monetary support for equipment (single crystal diffractometer, detector) and consumables from the ALS is substantially in excess of $300k. In addition to this monetary support, the ALS human infrastructure, in the form of software maintenance and development as well as many other necessary crafts, keeps the beamline in an operational state and allows for expansions of capabilities.

2015-16 Requested Budget

PI:	Williams, Quentin
Title:	COMPRES Year 5
Agency:	University of New Mexico

Project Start Date:	06/01/16	Project End Date:	05/31/17

Number of Periods:	1		
Project Location:	Off-Campus		
IDC Rate:	26.0%	IDC Type:	MTDC

Cayuse Proposal Number:	00-4218/Project A00-1520		
Preparer:	Heidi Gomez		
Budget Prepared Date:	10/26/15	Revised Date:	

UCSC Detailed Budget

					Period 1	Total
				Start Date:		
				End Date:		
Salary Information		Click here to add salary & fringe information				
Name	Title		Appt Type	Level		
Beavers, Christine	Asst. Researcher		RESASST	5	$92,185	$92,185
COL Increase (initial/annual)	3%	3%		Months/Time %	12 100%	
Yan, Jinyuan	Assoc. Project Scientist		ProjSciAssoc	3	$76,220	$76,220
COL Increase (initial/annual)	3%	3%		Months/Time %	12 100%	
COMPRES Match ALS Doctoral Fellow	GSR (Academic)		GSR-Res	6	$789	$789
COL Increase (initial/annual)				Months/Time %	1 18%	
COMPRES Match ALS Doctoral Fellow	GSR (Summer)		GSR-Res	6	$2,235	$2,235
COL Increase (initial/annual)				Months/Time %	3 17%	
				Total Salary	**$171,429**	**$171,429**
Fringe Information						
Name	Title		Appt Type	Level		
Beavers, Christine	Asst. Researcher		RESASST	5	$38,718	$38,718
Fringe %	42.00%			Override		
Yan, Jinyuan	Assoc. Project Scientist		ProjSciAssoc	3	$44,970	$44,970
Fringe %	59.00%			Override		
COMPRES Match ALS Doctoral Fellow	GSR (Academic)		GSR-Res	6	$20	$20
Fringe %	2.50%			Override		
COMPRES Match ALS Doctoral Fellow	GSR (Summer)		GSR-Res	6	$56	$56
Fringe %	2.50%			Override		
				Total Fringe	**$83,764**	**$83,764**
				Total Salary and Fringe	**$255,193**	**$255,193**
Domestic Travel Information						
Name	Destination					

Revised - 10/5/15

			$4,000	$4,000
				$0
		Total Domestic Travel	**$4,000**	**$4,000**
Foreign Travel Information				
Name	Destination			
	ACA Meeting		$2,000	$2,000
				$0
		Total Foreign Travel	**$2,000**	**$2,000**
Permanent Equipment				
Description				
				$0
				$0
				$0
				$0
				$0
		Total Equipment	**$0**	**$0**
Participant Support				
Type	Description			
Select One				$0
Select One				$0
		Total Participant Support	**$0**	**$0**
Subcontracts				
Institution	Subcontract PI			
		Base		
		Indirect Costs		
		Total	$0	$0
		Base		
		Indirect Costs		
		Total	$0	$0
		Total Subcontracts	**$0**	**$0**
UC Multicampus				
Institution	Multicampus PI			
		Base		
		Indirect Costs		
		Total	$0	$0
		Base		
		Indirect Costs		
		Total	$0	$0
		Total UC Multicampus	**$0**	**$0**
Other Direct Costs				
Type	Description			
Materials & Supplies			$9,000	$9,000
Select One				$0

Revised - 10/5/15

			Total Other Direct Costs	**$9,000**	**$9,000**
Costs at Non-Std. Rates					
Type	Description		IC Rate		
Select One					$0
Select One					$0
			Total Non-Std Costs	**$0**	**$0**
			Tuition	$0	
			Graduate Student Health Insurance	$0	
			Graduate Student Fees	$0	
			Graduate Fee Override	$375	
			Total Graduate Fees	$375	$375
			Total Other Direct Costs including GSR Fees, Subcontracts, and MCA's	$9,375	$9,375
			Direct Costs Base	$270,568	
			Direct Cost Override		
			Total Direct Costs	**$270,568**	**$270,568**
			Indirect Cost Base	$270,193	
			Indirect Cost Base Override		
			Total Indirect Cost Base	$270,193	$270,193
			IC Rate	26.0%	
			Non-Standard Indirect Costs	$0	$0
			Total Indirect Costs	**$70,250**	**$70,250**
			Total Amount Requested	**$340,818**	**$340,818**
	UARC STI/Fee/ARP:	$0	$0	$0	
			Total Cost Share		$0
			Total Project Amount	**$340,818**	**$340,818**

NOTES:

Revised - 10/5/15

Appendix 1. Publications for 12.2.2 for 2014 & 2015

2014 Publications and Theses (23)

Refereed Journal Articles (22)

1. Abdul-Jabbar, N.M., B. Kalkan, G-Y. Huang, A.A. MacDowell, R. Gronsky, E.D. Bourret-Courchesne, and B.D. Wirth, "The role of stoichiometric vacancy periodicity in pressure-induced amorphization of the Ga_2SeTe_2 semiconductor alloy," *Applied Physics Letters* **105**, 051908 (2014). (doi:10.1063/1.4892549)
2. Adcock, C., E. Hausrath, P.M. Forster, O. Tschauner, and K. Sefein, "Synthesis and characterization of the Mars-relevant phosphate minerals Fe- and Mg-whitlockite and merrillite and a possible mechanism that maintains charge balance during whitlockite to merrillite transformation ," *American Mineralogist* **99**(7), 1221-1232 (2014). (doi:10.2138/am.2014.4688)
3. An, K., S. Alayoglu, N. Musselwhite, K. Na, and G.A. Somorjai, "Designed Catalysts from Pt Nanoparticles Supported on Macroporous Oxides for Selective Isomerization of n-Hexane,"*Journal of the American Chemical Society* **136**(19), 6830-6833 (2014). (doi:10.1021/ja5018656)
4. Bae, S., C. Meral, J.e. Oh, J. Moon, M. Kunz, and P.J.M. Monteiro, "Characterization of morphology and hydration products of high-volume fly ash paste by monochromatic scanning x-ray micro-diffraction (\u956#-SXRD)," *Cement and Concrete Research* **59**, 155-164 (May2014). (doi:10.1016/j.cemconres.2014.03.001)
5. Bayarjargal, L., B. Winkler, A. Friedrich, and E.A. Juarez-Arellano, "Synthesis of TaC and Ta_2C from tantalum and graphite in the laser-heated diamond anvil cell," **59**(36), 5283-5289 (2014). (doi:10.1007/s11434-014-0546-5)
6. Chen, B., K.M. Lutker, J. Lei, J. Yan, S. Yang, and H. Mao, "Detecting Grain Rotation at the Nanoscale," *Proceedings of the National Academy of Sciences of the United States of America***111**(9), 3350-3353 (2014). (doi:10.1073/pnas.1324184111)
7. Fischer, R.A., A.J. Campbell, R. Caracas, D.M. Reaman, D.L. Heinz, P. Dera, and V.B. Prakapenka, "Equations of state in the Fe-FeSi system at high pressures and temperatures,"*Journal of Geophysical Research-Solid Earth* **119**(4), 2810-2827 (2014). (doi:10.1002/2013JB010898)
8. Hargis, C.W., J. Moon, B. Lothenbach, F. Winnefeld, H. Wenk, and P.J.M. Monteiro, "Calcium Sulfoaluminate Sodalite ($Ca_4Al_6O_{12}SO_4$) Crystal Structure Evaluation and Bulk Modulus Determination," *Journal of the American Ceramic Society* **97**(3), 892-898 (2014). (doi:10.1111/jace.12700)

9. Kalkan, B., R.P. Dias, C.S. Yoo, S.M. Clark, and S. Sen, "Polyamorphism and Pressure-Induced Metallization at the Rigidity Percolation Threshold in Densified $GeSe_4$ Glass,"*Journal of Physical Chemistry C* **118**(10), 5110-5121 (2014). (doi:10.1021/jp4108602)
10. Melaet, G.M., W.T. Ralston, C.S. Li, S. Alayoglu, K. An, N. Musselwhite, B. Kalkan, and G.A. Samorjai, "Evidence of Highly Active Cobalt Oxide Catalyst for the Fischer-Tropsch Synthesis and CO_2 Hydrogenation," *Journal of the American Chemical Society* **136**(6), 2260-2263 (2014). (doi:10.1021/ja412447q)
11. Moon, J., S. Bae, K. Celik, S. Yoon, K.H. Kim, K.S. Kim, and P. Monteiro, "Characterization of natural pozzolan-based geopolymeric binders," *Cement and Concrete Composites* **53**, 97-104 (October 2014). (doi:10.1016/j.cemconcomp.2014.06.010)
12. Musaev, O.R., J. Yan, V. Dusevich, J.M. Wrobel, and M.B. Kruger, "Ni nanoparticles fabricated by laser ablation in water," *Applied Physics A: Materials Science & Processing***116**(2), 735-739 (2014). (doi: 10.1007/s00339-014-8569-y)
13. O'Bannon, E., C.M. Beavers, and Q. Williams, "Trona at extreme conditions: A pollutant-sequestering material at high pressures and low temperatures," *American Mineralogist* **99**(10), 1973-1984 (2014). (doi:10.2138/am-2014-4919)
14. Rainey, E.S.G., and A. Kavner, "Peak scaling method to measure temperatures in the laser-heated diamond anvil cell and application to the thermal conductivity of MgO," *Journal of Geophysical Research-Solid Earth* **119**(11), 8154-8170 (2014). (doi:10.1002/2014JB011267)
15. Raju, S.V., Z.M. Geballe, B.K. Godwal, B. Kalkan, Q. Williams, and R. Jeanloz, "High pressure and temperature structure of liquid and solid Cd: Implications for the melting curve of Cd," *Materials Research Express* **1**(4), 046502 (2014). (doi:10.1088/2053-1591/1/4/046502)
16. Tan, D., W. Zhou, W. Ouyang, Z.M. Mi, L. Kong, W. Xiao, K. Zhu, and B. Chen, "Growth of magnesium aluminate nanocrystallites," *CrystEngComm* **16**, 1579-1583 (2014). (doi:10.1039/c3ce41718b)
17. Tongay, S., H. Sahin, C. Ko, A. Luce, W. Fan, K. Liu, J. Zhou, Y. Huang, C. Ho, J. Yan, D. Ogletree, S. Aloni, J. Ji, S. Li, J. Li, F. Peeters, and J. Wu, "Monolayer behaviour in bulk ReS_2 due to electronic and vibrational decoupling," *Nature Communications* **5**(6252), 1 (2014). (doi:10.1038/ncomms4252)
18. Tu, V., E. Hausrath, O. Tschauner, V. Iota, and G.W. Egeland, "Dissolution rates of amorphous Al- and Fe-phosphates and their relevance to phosphate mobility on Mars ,"*American Mineralogist* **99**(7), 1206 (2014). (doi:10.2138/am.2014.4613)
19. Wang, S., J. Zhang, J. Yan, X.J. Chen, V. Struzhkin, W. Tabis, N. Barisic, M.K. Chan, C. Dorrow, X. Zhao, M. Greven, W.L. Mao, and T. Geballe, "Strain derivatives of Tc in $HgBa_2CuO_4$: The CuO_2 plane alone is not enough," *Physical Review B: Condensed Matter and Materials Physics* **89**, 024515 (2014). (doi:10.1103/PhysRevB.89.024515)

20. Wenk, H-R., L. Lutterotti, P. Kaercher, W. Kanitpanyacharoen, L. Miyagi, and R. Vasin, "Rietveld texture analysis from synchrotron diffraction images. II. Complex multiphase materials and diamond anvil cell experiments," *Powder Diffraction* **29**(3), 220-232 (2014). (doi:10.1017/S0885715614000360)
21. Xie, M., R. Mohammadi, C.L. Turner, R.B. Kaner, A. Kavner, and S.H. Tolbert, "Lattice stress states of superhard tungsten tetraboride from radial x-ray diffraction under nonhydrostatic compression," *Physical Review B: Condensed Matter and Materials Physics***90**, 104104 (2014). (doi:10.1103/PhysRevB.90.104104)
22. Yang, F., Y. Lin, J.E.P Dahl, R.M.K Carlson, and W.L. Mao, "Deviatoric stress-induced phase transitions in diamantane," *Journal of Chemical Physics* **141**(15), 154305 (2014). (doi:10.1063/1.4897252)

Refereed Conference Proceedings (0)

Theses (M.S., Ph.D., etc.) (1)

1. Lerch, Andrew.T, "Synthesis, Structure, and Properties of Refractory Hard-Metal Borides," doctoral dissertation, University of California, Los Angeles, CA, 2014, advisor Richard B. Kaner.

Non-refereed Publications (magazine article, book review, etc.)(0)

2015 Publications and Theses to Date (18)

Refereed Journal Articles (18)

1. Baumeister, Julie.L., Elisabet Hausrath, Amanda A Olsen, Oliver Tschauner, Christop Adcock, and Rodney V Metcalf, "Biogeochemical weathering of serpentinites; An examination of incipient dissolution affecting serpentine soil formation," *Applied geochemistry* **54**, 74-84 (2015). (doi:dx.doi.org/10.1016/j.apgeochem.2015.01.002)
2. Boulard, E., A.F. Goncharov, M. Blanchard, and W. Mao, "Pressure induced phase transition in $MnCO_3$ and its implications on the deep carbon cycle," *Journal of Geophysical Research-Solid Earth*, 1 (2015). (doi:10.1002/2015JB011901)
3. Du, W., S.M. Clark, and D. Walker, "Thermo-compression of pyrope-grossular garnet solid solutions: Non-linear compositional dependence," *American Mineralogist* **100**(1), 215-222 (2015). (doi:http://dx.doi.org/10.2138/am-2015-4752)
4. Geng, G., R. Taylor, S. Bae, D. Hernandez-Cruz, D.A. Kilcoyne, A. Emwas, and P.J. Monteiro, "Atomic and nano-scale characterization of a 50-year-old hydrated C_3S paste," *Cement and Concrete Research* **77**, 36-46 (2015).

(doi:10.1016/j.cemconres.2015.06.010)

5. Jaffe, A., Y. Lin, W.L. Mao, and H.I. Karunadasa, "Pressure-Induced Conductivity and Yellow-to-Black Piezochromism in a Layered Cu-Cl Hybrid Perovskite," *Journal of the American Chemical Society* **137**(4), 1673-1678 (2015). (doi:10.1021/ja512396m)
6. Ma, C., O. Tschauner, J.R. Beckett, Y. Liu, G.R. Rossman, K. Zhuravlev, V. Prakapenka, P. Dera, and L.A. Taylor, "Tissintite, (Ca, Na, □)$AlSi_2O_6$, a highly-defective, shock-induced, high-pressure clinopyroxene in the Tissint martian meteorite," *Earth and Planetary Science Letters* **422**, 194-205 (2015). (doi:doi:10.1016/j.epsl.2015.03.057)
7. Marquardt, H., and L. Miyagi, "Slab stagnation in the shallow lower mantle linked to an increase in mantle viscosity," *Nature Geoscience* **8**, 311-314 (2015). (doi:doi:10.1038/ngeo2393)
8. Moon, J., S. Yoon, and P.JM. Monteiro, "Mechanical properties of jennite: A theoretical and experimental study," *Cement and Concrete Research* **71**, 106-114 (2015). (doi:doi:10.1016/j.cemconres.2015.02.005)
9. Raju, S.V., A.A. Oni, B.K. Godwal, J. Yan, V. Drozd, S. Srinivasan, J.M. Lebbeau, K. Rajan, and S.K. Saxena, "Effect of B and Cr on elastic strength and crystal structure of Ni_3Al alloys under high pressure," *Journal of Alloys and Compounds* **619**, 616-620 (January 2015). (doi:10.1016/j.jallcom.2014.09.012)
10. Rodenbough, P.R., J. Song, D. Walker, S.M. Clark, B. Kalkan, and S.W. Chan, "Size dependent compressibility of nano-ceria: Minimum near 33 nm," *Applied Physics Letters***106**, 163101 (2015). (doi:http://dx.doi.org/10.1063/1.4918625)
11. Serdar, M., C. Meral, M. Kunz, D. Bjegovic, H.-R. Wenk, and P.J.M. Monteiro, "Spatial distribution of crystalline corrosion products formed during corrosion of stainless steel in concrete," *Cement and Concrete Research* **71**, 93-105 (May 2015). (doi:10.1016/j.cemconres.2015.02.004)
12. Solis-Ibarra, D., C. Smith, and H.I. Karunadasa, "Post-synthetic halide conversion and selective halogen capture in hybrid perovskites," Chemical Science, 6, 4054-4059 (2015). (doi:10.1039/c5sc01135c)
13. Walker, D., J. Li, B. Kalkan, and S.M. Clark, "Thermal, compositional, and compressional demagnetization of cementite," *American Mineralogist* 100, 5306 (2015). (doi: http://dx.doi.org/10.2138/am-2015-5306)
14. Wisser, M.D., M. Chea, Y. Lin, D.M. Wu, W.L. Mao, A. Salleo, and J.A. Dionne, "Strain-Induced Modification of Optical Selection Rules in Lanthanide Based Upconverting Nanoparticles," *Nano Letters* **15**(3), 1891-1897 (2015). (doi:10.1021/nl504738k)
15. Xie, M., R. Mohammadi, C.L. Turner, R.B. Kaner, A. Kavner, and S.H. Tolbert, "Exploring hardness enhancement in superhard tungsten tetraboride-based solid solutions using radial X-ray diffraction," *Applied Physics Letters* **107**, 41903 (2015). (doi:10.1063/1.4927596)
16. Zeng, Z., Q. Zeng, N. Liu, A.R. Oganov, Q. Zeng, Y. Cui, and W.L. Mao, "A Novel Phase of $Li_{15}Si_4$ Synthesized under Pressure," *Advanced Energy Marterials* **5**, 1500214 (2015). (doi:10.1002/aenm.201500214)

17. Zhao, Z., Q. Zeng, H. Zhang, S. Wang, S. Hirai, Z. Zeng, and W.L. Mao, "Structural transition and amorphization in compressed α-Sb_2O_3," *Physical Review B: Condensed Matter and Materials Physics* **91**, 184114 (2015). (doi:10.1103/PhysRevB.91.184112)

18. Stavrou, Elissaio, M. Riad Manaa, Joseph M Zaug, I-Feng W Kuo, Philip F Pagoria, Bora Kalkan, Jonathan Crowhurst, and Michael Armstrong, "The high pressure structure and equation of state of 2,6-diamino-3,5-dinitropyrazine-1-oxide (LLM-105) up to 20 GPa: X-ray diffraction measurements and first principles molecular dynamics simulations," *Journal of Chemical Physics* **143**(14), 144506 (2015). (doi:10.1063/1.4932683)

Refereed Conference Proceedings (0)

Theses (M.S., Ph.D., etc.) (0)

Non-refereed Publications (magazine article, book review, etc.)(0)

Appendix 2. Successful Proposals & their allocated Beamtime

August –December 2014

ALS Shifts Allocation (2014-2 August - December)

Investigator	Title	Organization	BL	Final Rating	Shf Req	Shf Alloc	Shf Tot
Lavina, B	High Pressure Study of Fe4O5	University of Nevada Las Vegas	12.2.2		9	9	9
Ciezak-Jenkins, J	High-Pressure Single Crystal Diffraction of the Extended Solids of Carbon Monoxide and Nitrogen/Hydrogen Binary Mixtures	US Army Research Laboratory	12.2.2		12	12	21
Chen, B	Thermal equation of state of CaSiO3 perovskite under lower mantle conditions	University of Hawaii at Manoa	12.2.2		6	6	27
Karunadasa, H	Hybrid Materials for Anisotropic Compressibility and Reversible Piezochromism	Stanford University	12.2.2		12	12	39
Long, J	High-pressure synthesis and structural investigation of lanthanide diazenides	University of California Berkeley	12.2.2		12	12	51
Williams, Q	Resistive heating developments at BL 12.2.2 and its applications in axial and radial XRD experiments	University of California Santa Cruz	12.2.2		12	9	60
Dzivenko, D	High-pressure high-temperature synthesis of the ternary B-C-N systems	Technische Universität Darmstadt	12.2.2		9	9	69
Williams, Q	Single-Crystal X-ray Diffraction of Lawsonite and Topaz at Simultaneous High Pressures and Temperatu	University of California Santa Cruz	12.2.2		6	6	75
Williams, Q	Iron phase transition investigation at high temperature by laser heating at beamline 12.2.2	University of California Santa Cruz	12.2.2		9	9	84
Tolbert, S	HIGH PRESSURE STUDIES OF ULTRA-INCOMPRESSIBLE, SUPERHARD METALS	University of California Los Angeles	12.2.2		18	15	99
Mao, W	Study on pressure induced "superlubric" transition and metallization in MoSe2	Stanford University	12.2.2		6	6	105
Tschauner, O	Single Crystal Diffraction under Extreme Conditions	University of Nevada Las Vegas	12.2.2		12	12	117
Miyagi, L	Deformation and Texture Development of post-Perovskite Analogs	University of Utah	12.2.2		12	12	129
McCluskey, M	Phase transformations of In2Se3 under pressure	Washington State University	12.2.2		12	12	141
Jeanloz, R	Multi-ferropericlase single-crystal X-ray diffraction experiments at lower-mantle pressures	University of California Berkeley	12.2.2		12	12	153
Godwal, B	Structural and metallic phase transitions of PbCl2 and SnCl2 at pressures up to ~100 GPa.	University of California Berkeley	12.2.2		6	6	159
Mao, W	Study on Pressure Induced Structural Transitions in a proposed Dirac semi-metal Na3Bi	Stanford University	12.2.2		6	6	165
Godwal, B	Melting curve and structure of amorphous and liquid AuIn2 at high pressures	University of California Berkeley	12.2.2		12	9	174
Monteiro, P	Atomistic structures and structural mechanism of amorphous alkali-silicate reaction gel	University of California Berkeley	12.2.2		6	6	180
Clearfield, A	Structural investigation of metal phosphonates under applied pressure	Texas A&M University	12.2.2		3	3	183
Crowhurst, J	In situ x-ray diffraction study of the decomposition products of high nitrogen content precursors	Lawrence Livermore National Laboratory	12.2.2		3	3	186
Kumar, R	High pressure structural studies on Ge2Sb2Te5 at high temperatures	University of Nevada Las Vegas	12.2.2		8	6	192
deemyad, s	Structures of Lithium-rich intermetallics under pressure	University of Utah	12.2.2		5	4	196

14 Proposals of the 37 submitted were not allocated time during this period. 196 shifts were available in the General User pool and 328 were requested (1.67 x oversubscribed). 129 shifts of GU time were allocated to COMPRES users, or 65.8%. 25 shifts were allocated to the HPSTAR approved program. 26 additional shifts are allocated for the ALS beamline scientist (13 shifts) or Director's Discretionary Time(13 shifts). The Kavner group was allocated 6 shifts of low-flux time (2-Bunch) in order to use the laser heating system.

January- June 2015

ALS Shifts Allocation (2015-1 Jan-Jun)

Investigator	Title	Organization	BL	Final Rating	Shf Req	Shf Alloc	Shf Tot
Ciezak-Jenkins, J	High-Pressure Single Crystal Diffraction of the Extended Solids of Carbon Monoxide and Nitrogen/Hydrogen Binary Mixtures	US Army Research Laboratory	12.2.2		9	9	9
Chen, B	Thermal equation of state of CaSiO3 perovskite under lower mantle conditions	University of Hawaii at Manoa	12.2.2		6	6	15
Karunadasa, H	Hybrid Materials for Anisotropic Compressibility and Reversible Piezochromism	Stanford University	12.2.2		12	12	27
Long, J	High-pressure synthesis and structural investigation of lanthanide diazenides	University of California Berkeley	12.2.2		6	6	33
Jackson, J	Spin crossover P-V-T equations of state for (Mg,Fe)O throughout Earth's mantle conditions	California Institute of Technology	12.2.2		18	18	51
Williams, Q	Resistive heating developments at BL 12.2.2 and its applications in axial and radial XRD experiments	University of California Santa Cruz	12.2.2		9	9	60
Williams, Q	Single-Crystal X-ray Diffraction of Lawsonite and Topaz at Simultaneous High Pressures and Temperatu	University of California Santa Cruz	12.2.2		6	9	69
Tolbert, S	HIGH PRESSURE STUDIES OF ULTRA-INCOMPRESSIBLE, SUPERHARD METALS	University of California Los Angeles	12.2.2		9	9	78
McCluskey, M	Pressure induced phase transitions in crystalline and amorphous In2Se3	Washington State University	12.2.2		12	12	90
Kavner, A	Thermal Expansion and Thermal Conductivity of Planetary Metals, Oxides, and Silicates	University of California Los Angeles	12.2.2		6	6	96
Alivisatos, P	Understanding the structural transformations of Pt-bimetallic alloys during Propane Dehydrogenation	University of California Berkeley	12.2.2		12	12	108
Mao, W	Study on pressure induced "superlubric" transition and metallization in MoSe2	Stanford University	12.2.2		6	6	114
Mi, Z	The weakening of olivine induced by water in the mantle	HPSTAR	12.2.2		6	6	120
Ross, N	High-Pressure Diffraction Analysis of a 3D Copper Carbonate Complex with Sodalite Topology	Virginia Polytechnic Institute and State University	12.2.2		6	6	126
Miyagi, L	Deformation and Texture Development of post-Perovskite Analogs	University of Utah	12.2.2		12	12	138
Mao, W	Strength Determination of Iron Compounds	Stanford University	12.2.2		6	6	144
Jeanloz, R	Multi-ferropericlase single-crystal X-ray diffraction experiments at lower-mantle pressures	University of California Berkeley	12.2.2, 12.2.2		12	12	156
Godwal, B	Structural and metallic phase transitions of PbCl2 and SnCl2 at pressures up to ~100 GPa.	University of California Berkeley	12.2.2		12	12	168
Ciezak-Jenkins, J	High-Pressure Behavior of Extended Solids of Carbon Monoxide and Nitrogen Confined within Nanoporous Media	US Army Research Laboratory	12.2.2		6	6	174
Godwal, B	Structural and metallic phase transitions of BaCl2 and BaBr2 at pressures up to ~100 GPa.	University of California Berkeley	12.2.2		12	12	186
Sun, H	Synchrotron scattering study on Li0.8Fe0.2(OH)FeSe under pressure	University of California Berkeley	12.2.2		1	3	189
Levy, D	study of the effect of the pressure on 5-aminoterazole (5-AT) and its nitro salt: 5-aminoterazolium	Tel Aviv University	12.2.2		6	6	195
Forster, P	Pressure induced phase transitions in transition metal oxides	University of Nevada Las Vegas	12.2.2		9	9	204
Williams, Q	Characterization of laser heating at beamline 12.2.2 by iron phase transition investigation	University of California Santa Cruz	12.2.2		9	12	216

ALS Shifts Allocation (2015-1 Jan-Ju

Investigator	Title	Organization	BL	Shf Req	Shf Alloc	Shf Tot
Deemyad, S	Structures of organo alkali metal compounds under pressure	University of Utah	12.2.2	8	9	225

4 Proposals of the 29 submitted were not allocated time during this period. 225 shifts were available in the General User pool and 249 were requested (1.11 x oversubscribed). 130 shifts of GU time were allocated to COMPRES users, or 57.7%. 34 shifts were allocated to the HPSTAR approved program. 48 additional shifts are allocated for the ALS beamline scientist (18 shifts) or Director's Discretionary Time (30 shifts), of which, 9 shifts were dedicated to radiant heating commissioning experiments with Lukas Schlicker from TU Darmstadt.

July 2015-January 2016

ALS Shifts Allocation (2015-2 Jul - Dec)

Investigator	Title	Organization	BL	Final Rating	Shf Req	Shf Alloc	Shf Tot
Stavrou, E	X-ray diffraction study of alkali metal azides under high pressure and temperature conditions.	Lawrence Livermore National Laboratory	12.2.2		9	9	9
Ciezak-Jenkins, J	High-Pressure Single Crystal Diffraction of the Extended Solids of Carbon Monoxide and Nitrogen/Hydrogen Binary Mixtures	US Army Research Laboratory	12.2.2		9	9	18
Chen, B	Thermal equation of state of CaSiO3 perovskite under lower mantle conditions	University of Hawaii at Manoa	12.2.2		12	12	30
Miyagi, L	In-situ double sided laser heating and radial diffraction of lower mantle mineral phases	University of Utah	12.2.2		12	12	42
Williams, Q	Resistive heater developments at BL 12.2.2 and its high temperature and high pressure applications	University of California Santa Cruz	12.2.2		9	9	51
Santamaria-Perez, D	Synthesis and XRD study of high pressure-high temperature tetrahedrally-coordinated carbonates	Universidad de Valencia	12.2.2		9	9	60
Long, J	High-pressure synthesis and structural investigation of lanthanide diazenides	University of California Berkeley	12.2.2		6	6	66
Jackson, J	Spin crossover P-V-T equations of state for (Mg,Fe)O throughout Earth's mantle conditions	California Institute of Technology	12.2.2		18	15	81
Olmstead, M	Exploring Fullerenes Under Pressure	University of California Davis	12.2.2		6	6	87
Yaghi, O	Study of zeolitic imidazolate frameworks in variation of hydrostatic pressure	University of California Berkeley	12.2.2		12	9	96
Williams, Q	Single-Crystal X-ray Diffraction of Lawsonite and Topaz at Simultaneous High Pressures and Temperatu	University of California Santa Cruz	12.2.2		9	9	105
Tolbert, S	HIGH PRESSURE STUDIES OF ULTRA-INCOMPRESSIBLE, SUPERHARD METALS	University of California Los Angeles	12.2.2		9	9	114
McCluskey, M	Pressure induced phase transitions in crystalline and amorphous In2Se3	Washington State University	12.2.2		12	12	126
Kavner, A	Thermal Expansion and Thermal Conductivity of Planetary Metals, Oxides, and Silicates	University of California Los Angeles	12.2.2		9	9	135
Wenk, H	Rheology in the Earth's mantle: deformation of silicate perovskite + periclase	University of California Berkeley	12.2.2		9	9	144
Alivisatos, P	Understanding the structural transformations of Pt-bimetallic alloys during Propane Dehydrogenation	University of California Berkeley	12.2.2		12	9	153
Mao, W	Study on pressure induced "superlubric" transition and metallization in MoSe2	Stanford University	12.2.2		6	6	159
Tschauner, O	Single Crystal Diffraction under Extreme Conditions	University of Nevada Las Vegas	12.2.2		6	6	165
Mi, Z	The weakening of olivine induced by water in the mantle	HPSTAR	12.2.2		6	6	171
Ross, N	High-Pressure Diffraction Analysis of a 3D Copper Carbonate Complex with Sodalite Topology	Virginia Polytechnic Institute and State University	12.2.2		6	6	177
Jeanloz, R	Multi-ferropericlase single-crystal X-ray diffraction experiments at lower-mantle pressures	University of California Berkeley	12.2.2		12	6	183
Stavrou, E	X-ray diffraction study of Iodine oxides and oxoacids under high pressure conditions	Lawrence Livermore National Laboratory	12.2.2		6	6	189
Karunadasa, H	Structural Insight into the Electronic Properties of Organic-Inorganic Hybrid Materials	Stanford University	12.2.2		15	7	196

30 Proposals of the 53 submitted were not allocated time during this period. 196 shifts were available in the General User pool and 461 were requested (2.35 x oversubscribed). 115 shifts of GU time were allocated to COMPRES users, or 58.7%. 14 shifts were allocated to the HPSTAR approved program. 36 additional shifts are allocated for the ALS beamline scientist (14 shifts) or Director's Discretionary Time(22 shifts).

Appendix 3: The beamtime schedules for the last year's cycles

BL 12.2.2 Operating Schedule, Advanced Light Source, LBNL

July - Dec 2014

Beamtime requests to aamacdowell@lbl.gov

Jul-14	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
0000-0900	S/T	S/T	S/T	H	S/T	S/T	S/T	S/T	BLC	BLC	U	LM	LM	LM	AP	LM	WM	WM	RW	RW	IT	I		MM	MM	MM	MM	MS	RW	RW	U
0900-1700	S/T	S/T	BLC	H	S/T	S/T	S/T	BLC	BLC	U	MIYAGI			AP	U	MAO-6		WENK			M	I	U	McCLUSKY			AP	WENK		U	U
1700-2400	S/T	S/T	BLC	H	S/T	S/T	S/T	BLC	BLC	U	LM	LM	LM	AP	LM	WM	WM	RW	RW	RW	I	S/T	MM	MM	MM	MM	AP	RW	RW	U	U
										2 BUNCH																					
Aug-14	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
0000-0900	U	QW	JC	IT	I	MS						AK	AP	AK	AK	SC	SC	IT	I		JL	JL	QW	OT	OT	AP	RJ	RJ	IHR	SD	MS
0900-1700	QW1	QW	JC	M	I	AP					AK	AP	AK	AK	SC	SC		M	I	U	JL	QW1	OT	OT	AP	JEANLOZ		IHR	DEEMYAD		AP
1700-2400	QW1	JC	JC	I	S/T	AP					AK	AP	AK	AK	SC	SC		I	S/T	JL	JL	QW1	OT	OT	AP	RJ	RJ	IHR	SD	SD	AP
Sep-14	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	
	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	
0000-0900	H	IT	I		JCJ	JCJ	JCJ	JCJ	AP	RJ	RJ	QW	ST	ST	IT	I		HPSTAR		H	H	HPST	MS	DD	JL	JL	HK	WM	WM	IT	
0900-1700	H	M	I	U	C-JENKINS			AP	JEANLOZ		QW	TOLBERT			M	I	U	HPS	CHEN		HPS	AP	DD	LONG		HK	MAO 4		IT	IT	
1700-2400	H	I	S/T	JCJ	JCJ	JCJ	JCJ	AP	RJ	RJ	QW	ST	ST	ST	I	S/T	HPSTAR		H	H	HPS	AP	DD	JL	JL	HK	WM	WM	IT	IT	
						User Meeting																									
Oct-14	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
	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	DD	W	Th	F
0000-0900	IT	MM	IHR		MM	IT	I	AP		IHR	IHR	OT	OT	MS	BL	BL	BL	AC	PM	IT	I	I	I	S/T	S/T	S/T		DH	QW	HK	MM
0900-1700	U	IHR	IHR	MM	PM	M	I	AP	U	IHR	OT	OT	AP	U	LAVINA		AC	PM	MM	M	I	I	I	S/T	S/T	S/T	DH	QW	HK	MM	WM
1700-2400	PM	IHR	IHR	MM	PM	I	S/T	AP	IHR	IHR	OT	OT	AP	BL	BL	BL	AC	PM	MM	I	I	I	S/T	S/T	S/T	S/T	DH	QW	HK	MM	WM
Nov-14	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	
	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	
0000-0900	WM6		AP	I		QW	HK	HPSTAR			AP	SB	SB	SB	RK	RK	IT	I	MS		BG1	BG1	SY	SY	BG2	BG2	H	H	X	X	
0900-1700	WM6	AP	M	I	QW	HK	HPSTAR			AP		BHAT		RK	RK	MM	M	I	AP	BG1	BG1	SY	SY	BG2	BG2	U	H	H	X	X	
1700-2400	WM6	AP	I	S/T	QW	HK	HPSTAR			AP	SB	SB	SB	RK	RK	MM	I	S/T	AP	BG1	BG1	SY	SY	BG2	BG2		H	H	X	X	
															AGU																
Dec-14	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	Sa	Su	M	T	W
0000-0900	IT	I			HK	ST	ST	ST	AP	HPSTAR	LM	LM	LM	LM	IT	MS		HPS	MM	QW	QW	QW2	AP	H	H	H	X	X	X	X	H
0900-1700	M	I	U	HK	U	TOLBERT		AP	HPSTAR		MIYAGI				M	AP	U	HPS	QW	QW	QW	DH	AP	H	H	H	X	X	X	X	H
1700-2400	I	S/T		HK	ST	ST	ST	AP	HPSTAR	LM	LM	LM	LM		S/T	AP	HPS	MM	QW	QW	QW	DH	AP	H	H	H	X	X	X	X	H

ALS beamline 12.2.2
Schedule Jan 2015 - June 2015

Jan-2015	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	H	I	I	I	I	I	I	I	S/T	S/T	S/T	S/T	BLC			AP-HP*			H	IT	I	AP	S.O.				MS				
0800-1600	H	I	I	I	I	I	I	I	S/T	S/T	S/T	BLC	M/C						H	M	I	AP	091W.Mao		6875	AP	IHR	DD	5879	046Kavner	
1600-2400	H	I	I	I	I	I	I	S/T	S/T	S/T	S/T	BLC							H	I	S/T	AP				AP					
																									McCluskey				Karunadas		

Feb-2015	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
	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		AP	I	S.O.					MS							H	IT	I	S.O.					MS				
0800-1600	AP	M	I	95QW	6888Alivisatos				AP	6688Mi		IHR	000Forster			H	M	I	7049Godwal			AP	M/C		DD	848Ciezak		
1600-2400	AP	I	S/T						AP							H	I	S/T				AP						

March-2015	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
	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	T
0000-0800		AP	I	S.O.						MS						IT	I	AP	S.O.					MS					IT	I
0800-1600	AP	M	I	DD	AP-HP*				AP	M/C	IHR	95QW	767Tolbert			M	I	AP	M/C	5879	2Lon	6875	AP	7188Ross			6741Jeanloz			M	I
1600-2400	AP	I	S/T						AP							I	S/T	AP					AP							I	S/T
																			JY in China												
																				Karunadas		McCluskey									

	JY China / MK va	MK vacation

April-2015	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
	W	Th	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
0000-0800	AP	S.O.					MS							I	S.O.						MS					AP	I	S.O.	
0800-1600	AP		2-bunch			AP		2-bunch					M	I		DD		DD	AP	080QW/JY				6ChenHaw	AP	M	I	HP*	5879
1600-2400	AP					AP							I	S/T			170W. Mao		AP						AP	I	S/T		
																														Karunadas

May-2015	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					AP	I	S.O.					MS						IT	I	S.O.					H	S/T	AP				
0800-1600	85Deemyad			AP	M	I	M/C	179Ciezak			AP		6841Jackson					M	I	DSchl		6310Godwal			H	AP	6290	DSchl	6682	IHR	6875
1600-2400				AP	I	S/T					AP							I	S/T						H	AP					
																				Schlicker D							QW/SXD		Long	McCluskey

June-2015	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
	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
0000-0800	AP	I	S.O.					SS	SS						IT	I	AP	S.O.					AP					MS	
0800-1600	M	I	M/C	DSchl	6995QW		5879	SS	6837Lew		DD		AP-HP*		M	I	AP		5966Miyagi			AP	M/C		IHR		90QW / SX	AP	6875	49Su
1600-2400	I	S/T						SS							I	S/T	AP					AP						AP		
			Schlicker D				Karunadas		DD-HP-*-Pei																				McCluskey	

JULY IS DRAFT ONLY

July-2015	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
	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	F
0000-0800			H	X	X	IT	I	AP	S.O.					AP						IT	I	S.O.					MS				
0800-1600			H	X	X	M	I	AP					AP							M	I					AP					
1600-2400		U7	H	X	X	I	S/T	AP					AP							I	S/T					AP					

ALS beamline 12.2.2
Schedule July 2015- Jan 2016
v 6.9.15

COMPRES

Jul-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
	W	Th	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
0000-0800	7149		H	X	X	IT	I	AP	s.o.					AP			SXD 6290		Yaghi 7350	IT	I	s.o.						MS			
0800-1600	Yaghi 7350		H	X	X	M	I	AP	IHR		Mi 6688		AP	m/c	SXD 6290	DD	SXD 6290		Yaghi 7350	M	I	m/c	7540 HK	Kavner 7046			AP	OT 6455	DD	JY 7346	IHR
1600-2400	7350		H	X	X	I	S/T	AP					AP							I	S/T						AP				
																					Karunadasa						Tschauner				

Aug-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
	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	I	AP							AP					IT	I	s.o.						MS					AP
0800-1600	Long 6682	MMO 7306	M	I	AP	2-Bunch					AP		2-Bunch				M	I	MMO 7306	HK 7540	Miyagi 7349			AP	7349	m/c	Alivisatos 6888			AP	M
1600-2400	6682	7306	I	S/T	AP						AP						I	S/T	7306	7540				AP						AP	I
		Olmstead																													

Sep-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
	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	I	s.o.					H	S/T	AP					DD	I	s.o.						MS				IT	I	AP		
0800-1600	I	HK	JY	DD			H	AP	DD	HP*				M	I	DD	McC 6875	Tolbert 6767		AP	HK 7540	LLNL 7309		IHR	McCluskey 6875		M	I	AP	
1600-2400	S/T	7540	7346				H	AP						I	S/T					AP							I	S/T	AP	

Oct-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
	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	s.o.					IT	IT	MS					s.o.							AP											
0800-1600	SXD 6290	Jackson 6841			IT	IT	AP	OT 6455	Ciezak 6179			M	m/c	Ross 7188		LLNL 7277				Long 6682	W.Mao 6170		Wenk 7493			Maintanence Shutdown					
1600-2400	6290				IT	IT	AP	6455				S/T								AP											

Users Mtg

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	Maintenance Shutdown																									H	H	X	X	
0800-1600																										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	Maintenance Shutdown														Maintenance Start-Up & Tune									H	H	X	X	H	H	H	H
0800-1600																								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	Maintenance Start-Up & Tune			BLC				BLC		m/c	DD	IHR	McCluskey 6875	H	IT	I	s.o.					MS						
0800-1600	H	X	X															H	M	I	JY 7346	Santamaria-Perez 7565		AP	Jeanloz 6741			Chen-Hawaii 6556		
1600-2400	H	X	X															H	I	S/T				AP							