Beamline 1222, ALS
2018 COMPRES Annual Report
November 2017 – October 2018
Prepared by Quentin Williams (with input from J. Yan)

Overview

The operations at beamline 12.2.2 have had another quite successful year. Our personnel on both the COMPRES and ALS side formed a cohesive, productive and support-oriented team, with the COMPRES funded staff members being Christine Beavers (until 10/15/18, as discussed below) and Jinyuan Yan, and the ALS funded personnel being Martin Kunz (Beamline Scientist) and Scientific Engineering Associate Andrew Doran. Beamline Manager Alastair MacDowell continues to be allocated at nominal time to 12.2.2, but his contributions to 12.2.2 now mostly involve high-level advice on complex beamline issues (often x-ray optics). Our publication output continues to be strong, with the past two years being our most productive on record, and our accessing of beamtime by COMPRES-related users has consistently run at around 62% of the available time in each cycle (not including the HPSTAR Approved Program, which continues to be considerably supported by COMPRES staff). As in past years, this percentage of shifts 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, with our gas-loading system and laser miller each being used extensively by users. We continue to provide a wide range of capabilities, including our single crystal x-ray diffraction systems (a single axis system on endstation 2, and our Stoe Stadi-vari Eulerian cradle diffractometer, positioned on endstation 1), conventional axial diffraction (including under laser heating), and radial diffraction (including under two-sided laser heating), and continued availability of/work on external heating capabilities at high pressures.

Scientific Highlights

Our first highlight is a high profile contribution that probes the microscopic manifestations of isotropic stress on a molecular sample with rigid units joined together by a highly compressible central unit (a "mechanophore"). H. Yan et al. (Sterically controlled mechanochemistry under hydrostatic pressure, *Nature* **554**, 505-510, 2018: authors include W. Mao) probe the bonding changes that take place as a consequence of the *hydrostatically-induced* anisotropic microscopic strain that is produced by the strength contrasts within their engineered molecules. Figure 1 (left) shows the molecular design: hard carborane ligands are juxtaposed with a squishy Cu_4S_4 ring. These so-called "molecular anvils" hammer down anisotropically on the ring under pressure, forcing the Cu-S angles to dramatically distort. This angular change (of course) has an electronic effect---the highest occupied molecular orbital associated with the Cu-S bond shifts its geometry/energy to become an anti-bonding orbital. The S thus transfers electron density to Cu, reducing it from Cu(I) to Cu(0)---and the Cu in turn politely forms Cu metal nanocrystals, producing amorphization of the whole mess (Figure 1, right: disordering initiates at 8 GPa, and amorphization is completed at 12 GPa). The upshot of this is the overarching net proposal that 'mechanochemistry' can be deployed to microscopically torture by design soft molecular units in ways that chemists and materials scientists previously could only dream of. The concept of molecular anvils does have potentially broad implications for both microscopic stress and the nature of pressure at the molecular length-scale.

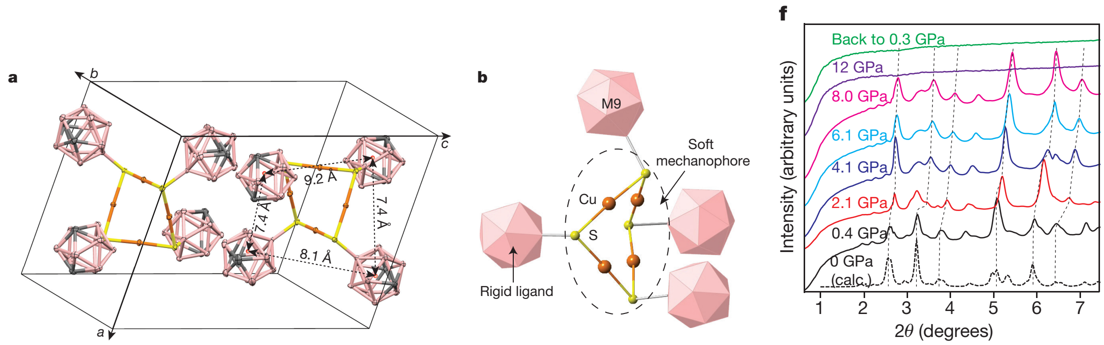

Figure 1. (left) Crystal structure and local structure of copper (I) m-carborane-9-thiolate crystals, and their diffraction pattern under pressure (right). From: H. Yan et al., Nature, 2018.

Our second highlight is chosen not only for its scientific interest, but also to illustrate the capabilities of our high-pressure single crystal x-ray diffraction system. Vennari et al. (JGR, 123, 6574-6591, 2018) probe the high pressure polymorphism of the alkali/calcium carbonate shortite ($Na_2Ca_2(CO_3)_3$): mantle carbonates have been shown to have frequent associations with alkali elements, and hence the phase equilibria of mixed alkali/alkaline earth carbonates has attracted considerable interest. Shortite, a phase observed as a product of carbonatite eruptions, was discovered to undergo multiple phase transitions under pressure. The first of these transitions, at ~15 GPa, is to a complex, low symmetry phase that was solved at 12.2.2. Figure 2 (left) shows the structure of the high-pressure monoclinic phase of shortite. But it is not simply the complexity of the structure that is notable: the single crystal solution gives fundamental insights into the shifting bonding of carbon under pressure in this phase. Figure 2 (right) shows a zoom-in of the bonding of two of the three carbon sites in the high-pressure phase (the locale of this configuration within the structure can be most easily seen above the two blue calcium cation sites on the left of the crystal structure). There is a nascent dimer formation between the two carbonate units: a configuration only previously observed in dolomite above ~65 GPa. In effect, the vauntedly stable isolated carbonate unit is approaching becoming a C_2O_6 unit. The underpinning importance of this observation, achievable only through high-quality high pressure single-crystal diffraction, is that carbonate units may distort and polymerize within complex structural environments at high pressures: hence, within complex, multi-cation phases or melts, dimerization of carbonate units may be a common occurrence under pressure.

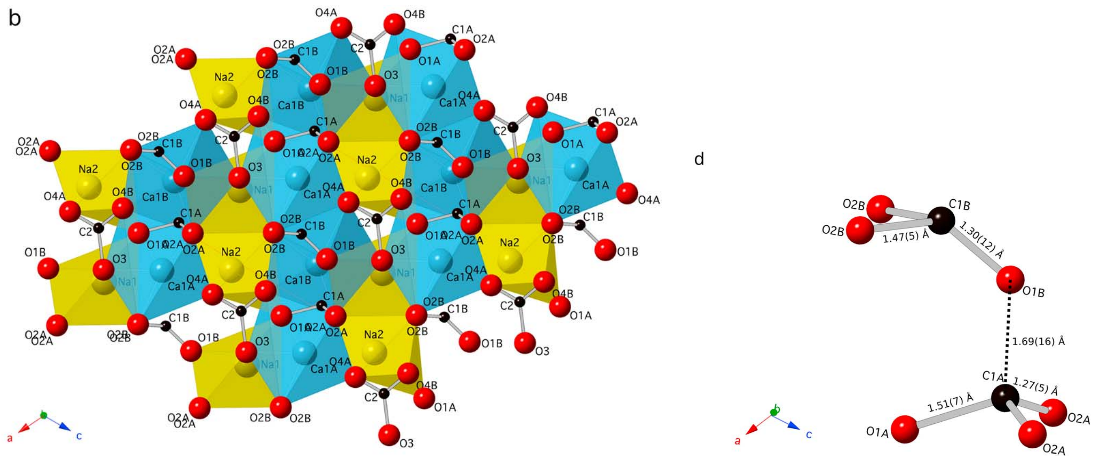

Figure 2. Crystal structure of a high-pressure phase of shortite (left), and carbon configuration of 2/3rds of the carbonate ions within the structure (right). From: Vennari et al., JGR, 2018.

Most years, one of our highlights is from a radial diffraction experiment to illustrate that particular capability of the beamline. We continue to emphasize radial diffraction at 12.2.2, but because of its provocative character, we instead highlight a study that deploys a machine-learning model to predict possible superhard materials, which were then synthesized and compressed at 12.2.2. Tehrani et al. (*Journal of the American Chemical Society* **140**, 9844-9853, 2018: authors include Miyagi) plug 2572 bulk and shear moduli of a bunch of compounds (probably 1286), their compositions, and their crystal structures into a machine-learning model, and turn the resultant rules loose on a database of 118,287 (!!) crystal structures. Two compounds (among others) emerged as possible real-stiff candidates: $ReWC_{0.8}$ and $Mo_{0.9}W_{1.1}BC$ (Fig. 3, left). Sure enough, when squeezed at 12.2.2, those two compounds did turn out to be epically stiff: a bulk modulus of 380 GPa for the ternary rhenium tungsten carbide, and 373 GPa for the quaternary molybdenum tungsten borocarbide. So, high-pressure diamond anvil cell measurements corroborated the machine-learning prediction of the bulk modulus, as well as confirmed the ultra-incompressible nature of both compounds.

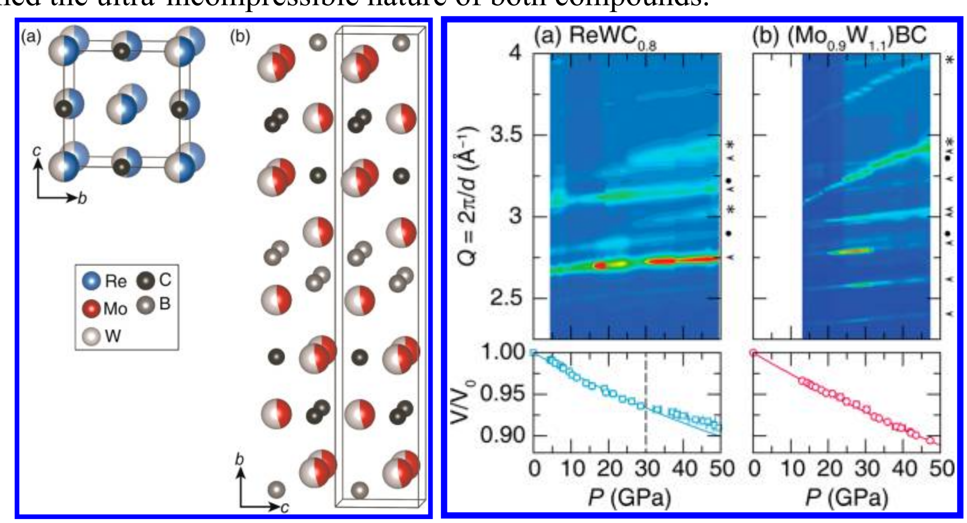

Figure 3 (left) Crystal structures of $ReWC_x$ and $Mo_{0.9}W_{1.1}BC$; and their diffraction patterns and equations of state (right). From: Tehrani et al., J.A.C.S. (2018).

Management Structure/Beamline Personnel

The core personnel responsible for beamline 12.2.2 has undergone a major change in the last month, although our organizational chart remains the same. Martin Kunz (with occasional consultation from Alastair MacDowell) is the ALS-employed beamline manager, and Andrew Doran provides half-time technical support to 12.2.2. Each of these folks is ALS funded, and their support at 12.2.2 is leveraged by the COMPRES investment. On the COMPRES side, Christine Beavers led the single-crystal high-pressure effort until her departure, and Jinyuan Yan continues to develop his respective projects and support the COMPRES community, as detailed in his individual annual report. The ALS staff report to MacDowell, the COMPRES staff report to Williams, but a formal dotted-line advising structure exists from Williams and MacDowell to each other's staff members. Other ongoing staffing includes an HPSTAR post-doc, Mingqiang Hou, who is specifically dedicated to helping HPSTAR users at 12.2.2.

Obviously, our major personnel shift was the departure of Christine Beavers to become the Principal Beamline Scientist at the high-pressure beamlines I15 and I15-1 at the Diamond Light Source in the U.K. In that role, she supervises five employees, and is charged with defining the directions and prioritizations at those beamlines. As such, while we regret her loss (and wish her well), this job change represented a very logical upward career move for her, and one that could not be accomplished within the COMPRES framework. Indeed, her effective promotion to full-scale Beamline head represents, in our view, one model career path for COMPRES employees: as she fully recognizes, COMPRES provided her with the opportunity to gain expertise in high-pressure science that augmented her formidable single-crystal diffraction expertise, and enabled her to move into a more responsible position. Her last day at the ALS was Oct. 15th--we had initially anticipated that she would continue through sometime between late Nov. and mid Dec. (and, quite frankly, take the lead on this report…), but her UK work visa appeared unexpectedly quickly, and she chose to depart at an earlier date.

A search is in progress for her replacement, and we have a strong applicant pool (the initial review date of the search was Nov. 8th, and creation of an interview shortlist is in progress: the search committee is Williams, Kunz and Kavner). We have 10 individuals with considerable high-pressure/synchrotron-oriented qualifications within the applicant pool. Relevant to this particular report, a portion of our applicant pool is quite experienced, and we are requesting funding that is comparable to what Beavers' salary would have been this year: this salary level is, given the Bay Area's cost of living, critical to recruit candidates at the more experienced end of our applicant pool.

Beamline Operations

Table 1. Beamtime Proposal Statistics at 12.2.2 for 2018 Beamline Cycles

<table>
<tr><td></td><td colspan="7">Jan. -June, 2018</td><td colspan="7">July -Dec. 2018</td></tr>
<tr><td># of beamtime proposals received</td><td colspan="7">76</td><td colspan="7">76</td></tr>
<tr><td># of beamtime proposals granted time</td><td colspan="7">30</td><td colspan="7">21</td></tr>
<tr><td>Total number of shifts requested</td><td colspan="7">664</td><td colspan="7">617</td></tr>
<tr><td>Total number of GU shifts granted</td><td colspan="7">253</td><td colspan="7">162</td></tr>
<tr><td>Total number of GU shifts available</td><td colspan="7">253</td><td colspan="7">162</td></tr>
<tr><td>Oversubscription rate</td><td colspan="7">2.6</td><td colspan="7">3.8</td></tr>
<tr><td># of visits by distinct research groups</td><td colspan="7">26*</td><td colspan="7">13* (in progress)</td></tr>
<tr><td rowspan="2">Number of unique users</td><td>Uni</td><td>Gov</td><td>Pri</td><td>USA</td><td>Can</td><td>Eur</td><td>Asi</td><td>Uni</td><td>Gov</td><td>Pri</td><td>USA</td><td>Can</td><td>Eur</td><td>Asi</td></tr>
<tr><td>27</td><td>6</td><td>0</td><td>19</td><td>1</td><td>6</td><td>7</td><td>11</td><td>4</td><td>0</td><td>13</td><td>0</td><td>0</td><td>2</td></tr>
<tr><td>Total number of person-visits</td><td colspan="7">126</td><td colspan="7">65 (in progress)</td></tr>
<tr><td>Number of undergraduate users</td><td colspan="7">2</td><td colspan="7">1</td></tr>
<tr><td>Number of graduate student users</td><td colspan="7">48</td><td colspan="7">21</td></tr>
<tr><td>Number of visits funded by each funding agency (NSF, DOD, DOE, Foreign/Other)</td><td colspan="7">See Table 2 Below</td><td colspan="7">See Table 2 Below</td></tr>
</table>

*The user office reports the number of distinct research groups for these spans of time at 12.2.2 as 33 and 15, respectively. The discrepancy with the number of Users in Table 2 below appears to be due to HPSTAR investigators belonging to multiple distinct research groups: Table 2 aggregates HPSTAR users.

The guidelines also request data on beamtime for two years: here are our beamline statistics from the two 2017 cycles from our 2017 Annual Report:
(1) Number of beamtime proposals received
Cycle 1-2017: 46
Cycle 2-2017: 64
(2) Number of beamtime proposals granted beamtime
Cycle 1-2017: 22,
Cycle 2-2017: 25
(3) Total number of shifts requested
Cycle 1-2017: 391
Cycle 2-2017: 529
(4) Total number of shifts granted
Cycle 1-2017: 187
Cycle 2-2017: 212
(5) Total number of shifts available
Cycle 1-2017: as (4): 187
Cycle 2-2017: as (4): 212
(6) Oversubscription rate (= shifts requested / shifts available)

Cycle 1-2017: 2.59
Cycle 2-2017: 2.67

Performance Metrics

Our spreadsheet for user statistics in the past year is below, and includes PI name, country, funding source, beamtime allocation, and total allocation of time to COMPRES users. Notably, all COMPRES user time at 12.2.2 is generated through the GU program (there is occasionally an award of the very limited Director's Discretionary time to COMPRES users, but this did not occur in these cycles). As described in the introduction (and within the spreadsheet), COMPRES users typically access ~60^{+}% of the available GU time, which is markedly in excess of the 35% of time that our Approved Program requires. There are two main nuances/ambiguities associated with these percentages. The first of these is: Who is a COMPRES user? For many users, this is unambiguous. But, there are investigators who reside in more of a gray area. Examples of these might include Stanford chemist H. Karunadasa, who collaborates with Wendy Mao on much of her high pressure research; UCLA chemist Sarah Tolbert, who collaborates with Abby Kavner on super-hard materials; and UCB chemist Jeffrey Long, who collaborates with Christine Beavers on catalytic sodalite structures. Because of the clear collaborations with COMPRES/Earth Sciences investigators, we included the former two in the COMPRES count, but not the last collaboration (in our view, this collaboration seemed largely like a binary chemist interaction). The second major nuance is whether HPSTAR time is included within the COMPRES inventory of time. We have chosen not to include it, since they have their own Approved Program, and a portion of their work is clearly out of the Earth Sciences domain. Moreover, we lack the knowledge to be able to assess which subsets of HPSTAR time are COMPRES-related, and which are entirely materials/chemistry/physics-oriented. Nevertheless, were HPSTAR (a foreign affiliate of COMPRES) included within our beamtime allocation statistics, our percentage of COMPRES-deployed beamtime would be substantially elevated.

Table 2: Users, Time Allotments, Affiliations and Funding Sources

ALS 12.2.2 Schedule 11/17-7/18

PI Last Name	PI First Name	Start Date	# of Shifts (3 = 1 day)	COMPRES User ©	Institution	Funding Source	Country	NSF-EAR	NSF-Material Science	NSF-CHE	DOE	DOD	NSERC-Canada	NSF-China
Williams	Quentin	11/3/17, 11/20, 3/17, 6/2	18	C	UCSC	NSF-EAR	USA	1						
Jackson	Jennifer	11/8/17	12	C	Caltech	NSF-EAR	USA	1						
Mao	Wendy	11/17/17,2/6, 4/20/18	21	C	Stanford-M	NSF-EAR/DMR, DOE	USA	1	1		1			
Monteiro	Paulo	12/1/17, 3/2/18	21	C	Berkeley-M	DOE	USA				1			
Stavrou	Elias	12/8/2017, 2/23/18	12	C	LLNL	DOE	USA				1			
Zeng	Q.	12/15/18	9		HPSTAR (GU)	Other (China)	China							
Ding	Y.	2/2/18	6		HPSTAR (GU)	Other (China)	China							1
Lee	Yongjae	2/8/18	3		South Korea (DD)	Other (South Korea)	S. Korea							1
Ciezak-Jenkins	Jennifer	2/9/18, 4/13/18, 6/29	18		Aberdeen Proving Grounds	ARO	USA					1		
Meshot	Eric	2/14, 6/20	6	C	LLNL	DOE	USA							
Karunadasa	H.	2/15, 3/14, 5/3, 6/21, 7/2	15	C	Stanford	NSF-DMR	USA		1					
Long	Jeffrey	12/10/17, 2/4, 2/25, 3/18	12		Berkeley-L	NSF-CHE	USA			1				
Miyagi	Lowell	3/7/18	12	C	Utah	NSF-EAR	USA	1						
Tschauner	Oliver	3/13/18	3	C	UNLV-P	NSF-EAR/DOE	USA	1			1			
Tolbert	Sarah	3/23/18	9	C	UCLA-T	NSF-DMR	USA		1					
Wenk	Hans-Rudolph	3/30/2018, 5/24	15	C	Berkeley-W	NSF-EAR	USA	1						
O'Bannon	Earl	5/10/2018, 6/14/18	6	C	LLNL	DOE	USA				1			
Shim	Sang-Heon	5/11/18	6	C	ASU	NSF-EAR	USA	1						
Zhou	X.	5/13/18, 6/10, 7/1	9		HPSTAR (GU)	Other (China)	China							1
Kavner	Abby	5/18/18	9	C	UCLA-K	NSF-EAR	USA	1						
Pravica	Michael	6/8/18	6		UNLV	DOE	USA				1			
Urban	Jeffrey	6/22/18	6		LBNL	DOE	USA				1			
Approved Program Time Allotments														
HPSTAR		Multiple	47+24 GU (above)		HPSTAR	China	China							
Gurlo		Multiple	27		TU-Berlin	FRG	Germany							
COMPRES			154					8	3	1	7	1		3
Total Shifts			234											

ALS 12.2.2 Schedule 8/1/18-11/1/18

PI Last Name	PI First Name	Start Date	# of Shifts (3 = 1 day)	COMPRES User ©	Institution	Funding Source	Country	NSF-EAR	NSF-Material Science	NSF-CHE	DOE	DOD	NSERC-Canada	NSF-China
Williams	Quentin	8/17, 10/1	6	C	UCSC	NSF-EAR	USA	1						
Monteiro	Paulo	10/4/18	6	C	Berkeley-M	DOE	USA				1			
Stavrou	Elias	9/6/18	3 (DD)	C	LLNL	DOE	USA				1			
Ciezak-Jenkins	Jennifer	9/7/2018, 10/23	12		Aberdeen Proving Grounds	ARO	USA					1		
Karunadasa	H.	8/17, 9/13, 10/19	9	C	Stanford	NSF-DMR	USA		1					
Long	Jeffrey	8/23, 10/18	6		Berkeley-L	NSF-CHE	USA			1				
Miyagi	Lowell	9/27/18	12	C	Utah	NSF-EAR	USA	1						
Tolbert	Sarah	8/31/18	8	C	UCLA-T	NSF-DMR	USA		1					
Wenk	Hans-Rudolph	9/21/18	9	C	Berkeley-W	NSF-EAR	USA	1						
O'Bannon	Earl	9/25/18	6	C	LLNL	DOE	USA				1			
Birgeneau	Bob	10/8/18	12		UCB/LBNL	NSF-DMR	USA		1					
Kavner	Abby	10/26/18	9	C	UCLA-K	NSF-EAR	USA	1						
Approved Program Time Allotments														
HPSTAR		Multiple	21			China	China							
Gurlo		None	0			FRG	Germany							
COMPRES			65											
Total Shifts			116											
						Total		4	3	1	3	1	0	0

Table 3: Beamtime allocations for the upcoming cycle, Jan. –June, 2019--Scheduling is in progress.

2019_1					
Investigator	Organization	**Shifts Alloc**	**Cumulative Shifts**	**COMPRES**	**Cumulative COMPRES**
Miyagi	University of Utah	12	12	12	12
Tolbert	University of California Los Angeles	9	21	9	21
Miyagi	University of Utah	12	33	12	33
Monteiro	University of California Berkeley	15	48	15	48
Wenk	Lawrence Berkeley National Laboratory	9	57	9	57
Chen	HPSTAR	9	66	0	57
Zhang	HPSTAR	3	69	0	57
Ciezak-Jenkins	US Army Research Laboratory	9	78	0	57
Godwal	University of California Berkeley	6	84	6	63
Zeng	HPSTAR	6	90	0	63
Yang	Southern University and A&M College	6	96	0	63
Chen	HPSTAR	6	102	0	63
Long	University of California Berkeley	9	111	0	63
Meshot	Lawrence Livermore National Laboratory	3	114	3	66
Mao	Stanford University	9	123	9	75
Karunadasa	Stanford University	9	132	9	84
Ewing	Stanford University	6	138	6	90
Wang	HPSTAR	9	147	0	90
Jeffries	Lawrence Livermore National Laboratory	6	153	6	96
Jeanloz	University of California Berkeley	9	162	9	105
Ding	HPSTAR	6	168	0	105
Gu	Stanford University	6	174	6	111
Chen	HPSTAR	6	180	0	111
Kavner	University of California Los Angeles	9	189	9	120
Lee	Yonsei University	6	195	0	120
Williams	University of California Santa Cruz	5	200	5	125

Beamline Community Activities

Among other professional activities, Christine Beavers served as an elected member on the ALS-wide Users Executive Committee (UEC), a body charged with providing advice and recommendations to the facility on behalf of the ALS user community, and served on the high pressure proposal review panel at the APS. The professional activities of the beamline scientists also included active engagement in a range of scientific meetings (at which an explicit goal is to promote the beamline, and its capabilities—these were, however, limited by our travel budget). It is probable that this coming year we will request that a high-pressure related workshop be conducted in conjunction with the ALS' annual user meeting: the precise topic will be decided on after input from our new staff member (we have had user meeting workshops about every 3-4 years, and it's time for another one).

Beamline Development

Over the past year, we completed a sequence of primarily software, but also some hardware modifications of our laser-heating system. In particular, our temperature measurement/pyrometry software was completely reconceptualized and redone. This was an extended joint effort between the ALS and COMPRES staff, and both the software and hardware developments are described in a very recent Review of Scientific Instruments paper (Kunz et al., Implementation and application of the peak scaling method for temperature measurement in the laser heated diamond anvil cell, *RSI* **89**, 083903, 2018). Our automated iterative technique to determine the sample peak temperature also allows quasi-real time temperature mapping of the laser-heated hot spot: importantly, these thermal maps are conducted without deploying any assumptions on shape, size and symmetry of the hot spot. Users have been quite enthusiastic about both the new pyrometry software and the stability of the new laser-heating system, and this year's essentially complete redoing of our pyrometry software formed an excellent tandem with last year's hardware rebuild of our laser-heating system.

During the July beam shutdown, considerable effort was also devoted to, during the July beam shutdown, characterizing the current state of the K-B mirrors on the beamline, in tandem with the ALS' x-ray optics group. While functional, they are relatively old and no longer fully optimal (as has long been known, and has been serially noted in past funding requests to COMPRES). The detailed characterization that took place fully documented their sub-optimality, and provided the quantitative documentation for a major request to the ALS for new K-B mirrors (discussed in the budget section below).

With respect to our single crystal diffraction systems, our primary development activities of the last year could loosely be described as being in an optimization/tune-up mode. Our external heating development enterprise (which is described in more detail in Yan's activity report) continued, with a range of heaters designed, tested and deployed.

The template query for this section also asks about "important problems or challenges" to the facility. There is a long-term prospective issue that we do not believe will be a problem (and actually might be an advantage), but which occupied a substantial amount of time over the last year in meeting attendance/written input/advocacy for Beavers, Kunz and Williams (to different degrees). The major ALS-U upgrade has progressed to CD-1 (see https://als.lbl.gov/wp-content/uploads/2018/09/Toward-a-New-Light_-Berkeley-Labs-ALS-Upgrade-Project-Moves-Forward.pdf for the press release on this). The possible concern for COMPRES down the line is that this project has been phrased as a largely soft X-ray focused enterprise—nevertheless, the hard X-ray beamlines are among the ALS' most scientifically productive beamlines (including 11.3.1 (small molecule crystallography), 12.2.2, 12.3.2 (microdiffraction) and so forth). The current management statement is that hard X-rays and superbends will definitely be present in the ALS-U, with probably a factor of ~6 greater brightness than the present ALS. There are technical challenges embedded within this intention; nevertheless, the upgrade could be a net advantage for high-pressure users. While this is not an urgent topic from the user perspective (ALS-U is in queue behind APS-U for upgrading, which puts the ALS upgrade likely into COMPRES-VI), the planning for this enterprise is accelerating, and the high-pressure enterprise at the ALS is certainly engaged in advocacy for a hard X-ray presence within ALS-U.

Planned Activities

Our planned activities in the coming year range from the comparatively routine to more ambitious goals that hinge upon the nature of, and skills of, our staffing moving forward. Among routine goals, the next logical step in cementing a fully user-friendly experience at 12.2.2 is to construct an improved off-line ruby fluorescence system. This is an occasional (but recurrent) request from users, and is a relatively straightforward exercise for which there are plans in place that simply need to be deployed (and, a few parts purchased). That's definitely in the routine category.

Our precise new initiatives for the coming COMPRES year hinge, to some extent, on the particular strengths of our new staff member. That said, we anticipate hiring someone with a significant level of single crystal experimental familiarity, in order to continue our momentum in this area. Given our tandem developments in, and focus on, external heating and single crystal x-ray diffraction, we believe we are at the cusp of making simultaneous high-pressure single-crystal/externally-heated experiments a non-heroic, and perhaps even routine, capability for users of 12.2.2: an intention of Beavers prior to her departure. In a different vein, given the ongoing maintenance, care and feeding of 12.2.2, our staff has not focused particularly on, nor promoted, inter-beamline projects---projects that are straightforward to facilitate at the ALS, given the ability to schedule synchronously (or sequentially) across beamlines. In this regard, the micro-Laue capabilities of 12.3.2 have been deployed on high-profile, high-pressure studies jointly with 12.2.2 (e.g., Friedrich et al., PRL,105, 085504, 2010), but tandem usage is rare. By the same token, the high-pressure infrared capabilities at 1.4.3, which underwent a resurgence during the NSLS infrared downtime, have been deployed seldomly of late (and there is certainly an advantage of nearly simultaneous infrared and X-ray experiments). Hence, a portion of the agenda of the new 12.2.2 staff member may be to work to enhance such cross-beamline studies within the community.

Budget

Staff: We request funding for two beamline scientists deployed for user support and instrumentation development from June 1, 2019 to May 31, 2020. This complement is viewed by ALS management as a match to the ALS staff that are deployed at 12.2.2, thus leveraging a substantial development and user support community. Jinyuan Yan is presently at the Associate Project Scientist III level. Dr. Beavers, our recently departed employee, was at the Associate Researcher II level, and had designed and developed the single-crystal capabilities at 12.2.2, as well as being the primary user support person for single-crystal diffraction experiments (and other users, as well). As described in the Introduction above, we aspire to be able to hire a beamline scientist at a similar level to Dr. Beavers, and believe that we have the applicant pool to do so; therefore, our salary request for this position is status quo from the past year (plus a standard 3% COL increase).

Dr. Yan provides software developmental work and day-to-day user support, and has worked on the development of external heating systems. His progress over the last year is described in more detail in his annual statements/inventory of work for COMPRES. Of key importance is that both employees are expected to routinely do a range of user-critical tasks at the beamline, such as maintenance and retuning of the off-line ruby fluorescence system, supporting users in the operation of the laser-miller and the gas-loader (or, more frequently, loading gases for users themselves, which ultimately usually saves time and cost), and a range of miscellaneous trouble-shooting associated with both our sample preparation lab and the beamline. Hence, this request represents *status quo* staffing of the facility moving forward.

Supplies and Expendables: A modest budget is requested for expendables utilized by COMPRES users at the beamline. This includes items such as replacement parts for equipment utilized by users (such as the gas-loading apparatus, the laser miller, sample preparation equipment, pressure measurement apparatus, gasket materials (boron, rhenium), and locally-made external heaters). The price of neon is also a contributor to this supply budget (ALS has usually generously supplied this but, given usage, the expectation is that COMPRES will buy in for a bottle in the not-too-distant future). With the increased percentage of COMPRES user time, our expendable budget allocation is under considerable strain.

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 US facilities to share best practices and to exchange expertise. We request a modest augmentation of this budget, since last year's allocation basically paid for participation in the COMPRES meeting and one other major trip.

Other Source of Beamline Funding: In terms of other sources of funding for the beamline, as discussed above, the deployment of two ALS-employed staff that devote very substantial portions of their time to assisting high-pressure geoscientists is a large-scale match for the COMPRES investment. The ALS has also, over the years, (among other things) invested in a gas-loader, multiple expensive detectors, and the Stoe diffractometer that is the centerpiece of our single-crystal enterprise. In the near term (as in very possibly this coming year), it is likely that the facility will invest in replacements for some of the rather old K-B mirrors on the beamline (there is a request in to the powers-that-be at the ALS, who concur that this is a priority for the beamline)---such a replacement would generate a notable improvement in our beam characteristics.

This Year's Proposed Budget:

NSF Budget Year 3

A. Senior Personnel			NSF Funded Person Months			Funds
			CAL	ACAD	SUM	
1.	TBD Asst./Assoc. Researcher		12	0	0	$102,060
2.	Jinyuan Yan		12	0	0	$87,200
3.			0	0	0	$0
4.			0	0	0	$0
5.			0	0	0	$0
6.	0	Others (list individually on budget explanation page)	0	0	0	$0
7.	0	Total Senior Personnel (1 through 6) 12	0	0	0	$0
B. Other Personnel						
1.	0	Post Doctoral Associates	0	0	0	$0
2.	0	Other Professional (Technician, Programmer, etc)	0	0	0	$0
3.		Graduate Students				$0
4.		Undergraduate Students				$0
5.	0	Secretarial-Clerical (if charged directly)				$0
6.	2	Other				$189,260
					Total Salaries and Wages (A+B)	$189,260
C. Fringe Benefits (If charged as direct costs)						$89,656
					Total Salaries, Wages and Fringe Benefits (A+B+C)	$278,916
D. Equipment (list item and dollar amount for each item exceeding $5,000)						
					Total Equipment	$0
E. Travel						
1. Domestic (Including U.S. Possessions)						$5,500
2. Foreign						$0
F. Participant Support						
1. Stipends		$0				
2. Travel		$0				
3. Subsistence		$0				
4. Other		$0				
		Total Participant Support				$0
G. Other Direct Costs						
1. Materials and Supplies						$4,000
2. Publication Costs/Documentation/Dissemination						$0
3. Consultant Services						$0
4. Computer Services						$0
5. Subawards						$0
6. Other						$0
					Total Other Direct Costs (G1 through G6)	$4,000
H. Total Direct Costs (A through G)						$288,416
I. Indirect Costs (F&A) (Specify Rate and Base)						
		26.0%	x	$288,416	Base	$74,988
J. Total Direct and Indirect Costs (H+I)						$363,404
K. Small Business Fee						
L. Amount of this request (J or J-K)						$363,404

And, Last Year's Budget, For Reference:

NSF Budget Year 2

A. Senior Personnel			NSF Funded Person Months CAL	ACAD	SUM	Funds
1.	Christine Beavers Assoc. Researcher II		0	0	0	$99,088
2.	Jinyuan Yan Assoc. Project Scientist		0	0	0	$83,387
3.			0	0	0	$0
4.			0	0	0	$0
5.			0	0	0	$0
6.	0	Others (list individually on budget explanation page)	0	0	0	$0
7.	2	Total Senior Personnel (1 through 6)	0	0	0	$182,475
B. Other Personnel						
1.	0	Post Doctoral Associates	0	0	0	$0
2.	0	Other Professional (Technician, Programmer, etc)	0	0	0	$0
3.		Graduate Students				$0
4.		Undergraduate Students				$0
5.	0	Secretarial-Clerical (if charged directly)				$0
6.	0	Other				$0
					Total Salaries and Wages (A+B)	$182,475
C. Fringe Benefits (If charged as direct costs)						$88,314
					Total Salaries, Wages and Fringe Benefits (A+B+C)	$270,789
D. Equipment (list item and dollar amount for each item exceeding $5,000)						
					Total Equipment	$0
E. Travel						
1. Domestic (Including U.S. Possessions)						$3,129
2. Foreign						$0
F. Participant Support						
1. Stipends		$0				
2. Travel		$0				
3. Subsistence		$0				
4. Other		$0				
		Total Participant Support				$0
G. Other Direct Costs						
1. Materials and Supplies						$3,300
2. Publication Costs/Documentation/Dissemination						$0
3. Consultant Services						$0
4. Computer Services						$0
5. Subawards						$0
6. Other						$0
					Total Other Direct Costs (G1 through G6)	$3,300
H. Total Direct Costs (A through G)						$277,218
I. Indirect Costs (F&A) (Specify Rate and Base)						
		26.0%	x	$277,218	Base	$72,077
J. Total Direct and Indirect Costs (H+I)						$349,295
K. Small Business Fee						
L. Amount of this request (J or J-K)						$349,295

User Satisfaction

The options available for user feedback at the ALS involve a multiple choice survey (which is reasonably frequently filled out by users): this survey has the option of giving more extended comments on each subtopic. The multiple choice survey includes both a sliding scale of satisfaction on a range of parameters, and a request that they check off the various benefits from their work at the ALS. The results, for the last year, of the multiple choice and benefits survey are given in the non-numbered table directly below. The more extended comments, of which there are relatively few, are given in Appendix 3.

For the dates of 10/1/2017 to 9/30/2018					
Total Questionnaires 31					
Question	very dissatisfied	dissatisfied	neither satisfied nor dissatisfied	satisfied	very satisfied
Accelerator beam delivered on schedule	0	0	2	8	21
Accelerator beam at specification	0	0	0	5	26
Beamline close to specification	0	2	0	7	22
ALSHUB User Portal and User Guide	0	0	4	12	15
Scientific and technical support (i.e. Beamline Scientists)	0	1	1	4	25
Scheduling of beamtime	0	0	1	9	20
Experiment proposal processing	0	0	1	11	17
Safety training	0	0	0	6	24
Amount of beamtime available annually	0	1	4	13	13
Overall experience at ALS	0	0	1	8	22
User Office Support and on-site registration	0	0	2	8	20
ALS Web Pages	0	0	5	10	13
Other Facility Support	0	0	1	6	18
Overall ALS Cleanliness	1	0	1	14	15
LBNL on-site Guest House	0	0	1	3	7
Benefits	# of Users checking Benefits Results				
Created new fundamental knowledge (i.e. basic research)	26				
Discovered other new knowledge (i.e. applied research)	10				
Developed a new or improved product, process or technology (i.e. development)	2				
Publication in peer-reviewed open literature	27				
Presentations at professional society meetings	16				
Other presentations	9				
Acquired a patent	0				
Obtained access to unique capabilities not available elsewhere	4				
Facilitated collaborative interactions	5				
Trained students (undergraduate, graduate or postdoctoral associate)	7				
Other benefit(s); Please specify	0				
Furthered Department of Energy missions	2				

Appendices

Appendix 1: Publication Lists for 2017 and 2018

2017 Publications and Theses (47)

Refereed Journal Articles (42)

1. Abramson, E.H., O. Bollengier, and J.M. Brown, "Water-carbon dioxide solid phase equilibria at pressures above 4 GPa," *Scientific Reports* **7**(1), 821 (2017). (doi:10.1038/s41598-017-00915-0) 12.2.2

2. Adcock, C.T., O. Tschauner, E.M. Hausrath, A. Udry, S.N. Luo, Y. Cai, M. Ren, A. Lanzirotti, M. Newville, M. Kunz, and C. Lin, "Shock-transformation of whitlockite to merrillite and the implications for meteoritic phosphate," *Nature Communications* **8**, 14667 (2017). (doi:10.1038/ncomms14667) 12.2.2

3. Bae, S., R. Taylor, D. Kilcoyne, J. Moon, and P. Monteiro, "Effects of Incorporating High-Volume Fly Ash into Tricalcium Silicate on the Degree of Silicate Polymerization and Aluminum Substitution for Silicon in Calcium Silicate Hydrate," *Materials* **10**(2), 131 (2017). (doi:10.3390/ma10020131) 5.3.2.1, 5.3.2.2, 12.2.2

4. Borstad, G.M., and J.A. Ciezak-Jenkins, "Hydrogen-Bonding Modification in Biuret Under Pressure," *Journal of Physical Chemistry A* **121**(4), 762-770 (2017). (doi:10.1021/acs.jpca.6b09670) 12.2.2

5. Cai, W., M. Dunuwille, J. He, T.V. Taylor, J.K. Hinton, M.C. MacLean, J.J. Molaison, A.M. Dos Santos, S. Sinogeikin, and S. Deemyad, "Deuterium Isotope Effects in Polymerization of Benzene under Pressure," *The Journal of Physical Chemistry Letters* **8**(8), 1856-1864 (2017). (doi:10.1021/acs.jpclett.7b00536) 12.2.2

6. Cai, W., R. Zhang, Y. Yao, and S. Deemyad, "Piezochromism and structural and electronic properties of benz[a]anthracene under pressure," *Phys. Chem. Chem. Phys.* **19**(8), 6216-6223 (2017). (doi:10.1039/C6CP08171A) 12.2.2

7. Chen, Y., F. Ke, P. Ci, C. Ko, T. Park, S. Saremi, H. Liu, Y. Lee, J. Suh, L.W. Martin, J.W. Ager, B. Chen, and J. Wu, "Pressurizing Field-Effect Transistors of Few-Layer MoS_2 in a Diamond Anvil Cell," *Nano Letters* **17**(1), 194-199 (2017). (doi:10.1021/acs.nanolett.6b03785) 12.2.2

8. Chen, Y., S. Zhang, F. Ke, C. Ko, S. Lee, K. Liu, B. Chen, J.W. Ager, R. Jeanloz, V. Eyert, and J. Wu, "Pressure-Temperature Phase Diagram of Vanadium Dioxide," *Nano Letters* **17**(4), 2512-2516 (2017). (doi:10.1021/acs.nanolett.7b00233) 12.2.2

9. Ci, P., Y. Chen, J. Kang, R. Suzuki, H.S. Choe, J. Suh, C. Ko, T. Park, K. Shen, Y. Iwasa, S. Tongay, J.W. Ager, L.-W. Wang, and J. Wu, "Quantifying van der Waals Interactions in Layered Transition Metal Dichalcogenides from Pressure-Enhanced Valence Band Splitting," *Nano Letters* **17**(8), 4982-4988 (2017). (doi:10.1021/acs.nanolett.7b02159) 12.2.2

10. Ciezak-Jenkins, J.A., and T.A. Jenkins, "Shear induced weakening of the hydrogen bonding lattice of the energetic material 5,5,Ä≤-Hydrazinebistetrazole at high-pressure," *J. Mol. Struct.* **1129**, 313-318 (2017). (doi:10.1016/j.molstruc.2016.09.084) 12.2.2

11. Ciezak-Jenkins, J.A., B.A. Steele, G.M. Borstad, and I.I. Oleynik, "Structural and spectroscopic studies of nitrogen-carbon monoxide mixtures: Photochemical response and observation of a novel phase," *The Journal of Chemical Physics* **146**(18), 184309 (2017). (doi:10.1063/1.4983040) 12.2.2

12. Ciezak-Jenkins, J.A., G.M. Borstad, and I.G. Batyrev, "Characterization of the Isothermal Compression Behavior of LLM-172," *Journal of Physical Chemistry A* **121**(22), 4263-4271 (2017). (doi:10.1021/acs.jpca.7b03300) 12.2.2

13. Doran, A., L. Schlicker, C.M. Beavers, S. Bhat, M.F. Bekheet, and A. Gurlo, "Compact low power infrared tube

furnace for in situ X-ray powder diffraction," *Rev. Sci. Instrum.* **88**(1), 013903 (2017). (doi:10.1063/1.4973561) 12.2.2

14. Vennari, C.E, E.F. O'Bannon, and Q. Williams, "The ammonium ion in a silicate under compression: infrared spectroscopy and powder X-ray diffraction of $NH_4AlSi_3O_8$--buddingtonite to 30 GPa," *Physics and Chemistry of Minerals* **44**(2), 149-161 (2017). (doi:10.1007/s00269-016-0844-3) 12.2.2

15. Geng, G., R.J. Myers, J. Li, R. Maboudian, C. Carraro, D.A. Shapiro, and P.M. Monteiro, "Aluminum-induced dreierketten chain cross-links increase the mechanical properties of nanocrystalline calcium aluminosilicate hydrate," *Scientific Reports* **7**, 44032 (2017). (doi:10.1038/srep44032) 5.3.2.1, 12.2.2

16. Geng, G., R.J. Myers, M.J. Qomi, and P. Monteiro, "Densification of the interlayer spacing governs the bynanomechanical properties of calcium-silicate-hydrate," *Scientific Reports* **7**(1), 10986 (2017). (doi:10.1038/s41598-017-11146-8) 12.2.2

17. Gomis, O., B. Lavina, P. Rodríguez-Hernández, A. Muñoz, R. Errandonea, D. Errandonea, and M. Bettinelli, "High-pressure structural, elastic, and thermodynamic properties of zircon-type $HoPO_4$ and $TmPO_4$," *Journal of Physics: Condensed Matter* **29**(9), 095401 (2017). (doi:10.1088/1361-648X/aa516a) 12.2.2

18. Groome, C., I. Roh, T.M. Mattox, and J.J. Urban, "Effects of Size and Structural Defects on the Vibrational Properties of Lanthanum Hexaboride Nanocrystals," *ACS Omega* **2**(5), 2248-2254 (2017). (doi:10.1021/acsomega.7b00263) 12.2.2

19. Hong, F., B. Yue, Z. Liu, B. Chen, and H.-K. Mao, "Pressure-driven semiconductor-semiconductor transition and its structural origin in oxygen vacancy ordered $SrCoO_{2.5}$," *Physical Review B* **95**(2), 024115 (2017). (doi:10.1103/PhysRevB.95.024115) 12.2.2

20. Jaffe, A., Y. Lin, W.L. Mao, and H.I. Karunadasa, "Pressure-Induced Metallization of the Halide Perovskite $(CH_3NH_3)PbI_3$," *Journal of the American Chemical Society* **139**(12), 4330-4333 (2017). (doi:10.1021/jacs.7b01162) 12.2.2

21. Kapustin, E.A., S. Lee, A.S. Alshammari, and O.M. Yaghi, "Molecular Retrofitting Adapts a Metal-Organic Framework to Extreme Pressure," *ACS Cent Sci* **3**(6), 662-667 (2017). (doi:10.1021/acscentsci.7b00169) 12.2.2

22. Köck, E.-M., M. Kogler, T. Götsch, L. Schlicker, M.F. Bekheet, A. Doran, A. Gurlo, B. Klötzer, B. Petermüller, D. Schildhammer, N. Yigit, and S. Penner, "Surface chemistry of pure tetragonal ZrO_2 and gas-phase dependence of the tetragonal-to-monoclinic ZrO_2 transformation," *Dalton Trans.* **46**(14), 4554-4570 (2017). (doi:10.1039/C6DT04847A) 12.2.2

23. Köck, E.-M., M. Kogler, C. Zhuo, L. Schlicker, M.F. Bekheet, A. Doran, A. Gurlo, and S. Penner, "Surface Chemistry and Stability of Metastable Corundum-Type In_2O_3," *Phys. Chem. Chem. Phys.* **19**(29), 19407-19419 (2017). (doi:10.1039/C7CP03632A) 12.2.2

24. Mattox, T.M., C. Groome, A. Doran, C.M. Beavers, and J.J. Urban, "Anion-mediated negative thermal expansion in lanthanum hexaboride," *Solid State Commun.* **265**, 47-51 (2017). (doi:10.1016/j.ssc.2017.07.012) 12.2.2

25. Nisr, C., Y. Meng, A.A. MacDowell, J. Yan, V. Prakapenka, and S.-H. Shim, "Thermal expansion of SiC at high pressure-temperature and implications for thermal convection in the deep interiors of carbide exoplanets," *Journal of Geophysical Research: Planets* **122**(1), 124-133 (2017). (doi:10.1002/2016JE005158) 12.2.2

26. O'Bannon, E.F., C.M. Beavers, M. Kunz, and Q. Williams, "The high-pressure phase of lawsonite: A single crystal study of a key mantle hydrous phase," **122**(8), 6294-6305 (2017). (doi:10.1002/2017JB014344) 11.3.1, 12.2.2

27. Raju, S.V., R. Hrubiak, V. Drozd, and S. Saxena, "Laser-assisted processing of Ni-Al-Co-Ti under high pressure," *Mater. Manuf. Processes* **32**(14), 1606-1611 (2017). (doi:10.1080/10426914.2016.1269913) 12.2.2

28. Rittman, D.R., S. Park, C.L. Tracy, L. Zhang, R.I. Palomares, M. Lang, A. Navrotsky, W.L. Mao, and R.C. Ewing, "Structure and bulk modulus of Ln-doped UO_2 (Ln = La, Nd) at high pressure," *Journal of Nuclear Materials* **490**, 28-33 (2017). (doi:10.1016/j.jnucmat.2017.04.007) 12.2.2

29. Rittman, D.R., K.M. Turner, S. Park, A.F. Fuentes, J. Yan, R.C. Ewing, and W.L. Mao, "High-pressure behavior of $A_2B_2O_7$ pyrochlore (A=Eu, Dy; B=Ti, Zr)," *J. Appl. Phys.* **121**(4), 045902 (2017). (doi:10.1063/1.4974871) 12.2.2

30. Rittman, D.R., K.M. Turner, S. Park, A.F. Fuentes, C. Park, R.C. Ewing, and W.L. Mao, "Strain engineered pyrochlore at high pressure," *Scientific Reports* **7**(1), 2236 (2017). (doi:10.1038/s41598-017-02637-9) 12.2.2

31. Rodenbough, P.P., and S.-W. Chan, "Crystallite-size dependency of the pressure and temperature response in nanoparticles of magnesia," *Journal of Nanoparticle Research* **19**(7), 241 (2017). (doi:10.1007/s11051-017-3922-7) 12.2.2

32. Ryu, Y.-J., C.-S. Yoo, M. Kim, X. Yong, J. Tse, S.K. Lee, and E.J. Kim, "Hydrogen-Doped Polymeric Carbon Monoxide at High Pressure," *Journal of Physical Chemistry C* **121**(18), 10078-1008 (2017). (doi:10.1021/acs.jpcc.7b01506) 12.2.2

33. Santamaría-Pérez, D., T. Marqueño, S. MacLeod, J. Ruiz-Fuertes, D. Daisenberger, R. Chuliá-Jordan, D. Errandonea, J.L. Jordá, F. Rey, C. McGuire, A. Mahkluf, A. Kavner, and C. Popescu, "Structural Evolution of CO_2-Filled Pure Silica LTA Zeolite under High-Pressure High-Temperature Conditions," *Chem. Mater.* **29**(10), 4502-4510 (2017). (doi:10.1021/acs.chemmater.7b01158) 12.2.2

34. Schlicker, L., M.F. Bekheet, and A. Gurlo, "Scaled-up solvothermal synthesis of nanosized metastable indium oxyhydroxide (InOOH) and corundum-type rhombohedral indium oxide (rh-In_2O_3)," *Z. Kristallogr.* **232**(1-3), 129-140 (2017). (doi:10.1515/zkri-2016-1967) 12.2.2

35. Slavney, A.H., R.W. Smaha, I.C. Smith, A. Jaffe, D. Umeyama, and H.I. Karunadasa, "Chemical Approaches to Addressing the Instability and Toxicity of Lead-Halide Perovskite Absorbers," *Inorganic Chemistry* **56**(1), 46-55 (2017). (doi:10.1021/acs.inorgchem.6b01336) 11.3.1, 12.2.2

36. Stavrou, E., J.M. Zaug, S. Bastea, and M. Kunz, "A study of tantalum pentoxide Ta_2O_5 structures up to 28 GPa," *J. Appl. Phys.* **121**(17), 175901 (2017). (doi:10.1063/1.4982708) 12.2.2

37. Steele, B.A., E. Stavrou, J.C. Crowhurst, J.M. Zaug, V.B. Prakapenka, and I.I. Oleynik, "High-Pressure Synthesis of a Pentazolate Salt," *Chem. Mater.* **29**(2), 735-741 (2017). (doi:10.1021/acs.chemmater.6b04538) 12.2.2

38. Turner, K.M., D.R. Rittman, R.A. Heymach, C.L. Tracy, M.L. Turner, A.F. Fuentes, W.L. Mao, and R.C. Ewing, "Pressure-induced structural modifications of rare-earth hafnate pyrochlore," *Journal of Physics: Condensed Matter* **29**(25), 255401 (2017). (doi:10.1088/1361-648X/aa7148) 12.2.2

39. Wicks, J., J.M. Jackson, W. Sturhahn, and D. Zhang, "Sound velocity and density of magnesiowüstites: Implications for ultralow-velocity zone topography," *Geophys. Res. Lett.* **44**(5), 2148-2158 (2017). (doi:10.1002/2016GL071225) 12.2.2

40. Zhang, F., Y. Wu, H. Lou, Z. Zeng, V.B. Prakapenka, E. Greenberg, Y. Ren, J. Yan, J.S. Okasinski, X. Liu, Y. Liu, Q. Zeng, and Z. Lu, "Polymorphism in a high-entropy alloy," *Nature Communications* **8**, 15687 (2017). (doi:10.1038/ncomms15687) 12.2.2

41. Zhou, X., N. Tamura, Z. Mi, J. Lei, J. Yan, L. Zhang, W. Deng, F. Ke, B. Yue, and B. Chen, "Reversal in the Size Dependence of Grain Rotation," *Physical Review Letters* **118**(9), 096101 (2017).

(doi:10.1103/PhysRevLett.118.096101) 12.2.2, 12.3.2

42. Zhu, W., G. Moore, B. Aitken, S. Clark, and S. Sen, "Observation of Steady Shear-Induced Nematic Ordering of Selenium Chain Moieties in Arsenic Selenide Liquids," *Journal of Physical Chemistry B* **121**(32), 7715-7722 (2017). (doi:10.1021/acs.jpcb.7b05115) 12.2.2

Refereed Conference Proceedings (2)

1. Götsch, T., C. Praty, M. Grünbacher, L. Schlicker, M.F. Bekheet, A. Doran, A. Gurlo, M. Tada, H. Matsui, N. Ishiguro, B. Kloetzer, and S. Penner, "Iron Exsolution Phenomena in Lanthanum Strontium Ferrite SOFC Anodes," *ECS Transactions* **78**(1), 1327-1341 (2017). [Proceedings of SOFC-XV: 15th International Symposium on Solid Oxide Fuel Cells, (Hollywood, FL, 2017)]. (doi:10.1149/07801.1327ecst) 12.2.2

2. Steele, B.A., E. Stavrou, V.B. Prakapenka, H. Radousky, J. Zaug, J.C. Crowhurst, and I.I. Oleynik, "Cesium pentazolate: A new nitrogen-rich energetic material," *AIP Conference Proceedings* **1793**, 040016 (2017). [Proceedings of American Physical Society Topical Group on Shock Compression of Condensed Matter, (Tampa Bay, Florida, 2015)]. (doi:10.1063/1.4971510) 12.2.2

Theses (M.S., Ph.D., etc.) (3)

1. O'Bannon, E.F., "High-pressure studies of subduction zone related mineral phases," Doctoral Dissertation, University of California Santa Cruz, Santa Cruz, CA, 2017, advisor Quentin Williams. 12.2.2, 11.3.1, 1.4

2. Zepeda-Alarcon, E., "Texture Development and Polycrystal Plasticity of Two-Phase Aggregates," Doctoral Dissertation, University of California, Berkeley, Berkeley, California, USA, 2017, advisor Hans-Rudolf Wenk. 12.2.2

3. Zhou, X., "Study on the plastic deformation and elastic properties of nano metal," Doctoral Dissertation, Center for High Pressure Science and Technology Advanced Research (HPSTAR), Shanghai, China, 2017, advisor Bin Chen. 12.2.2, 12.3.2

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

2018 Publications and Theses (37 to date)

Refereed Journal Articles (36 to date)

1. Bekheet, M.F., L. Schlicker, A. Doran, K. Siemensmeyer, and A. Gurlo, "Ferrimagnetism in manganese-rich gallium and aluminium spinels due to mixed valence Mn^{2+}–Mn^{3+} states," *Dalton Transactions* **47**(8), 2727-2738 (2018). (doi:10.1039/C7DT04765G) 12.2.2

2. Batyrev, I.G., S.P. Coleman, J. Ciezak-Jenkins, E. Stavrou, and J.M. Zaug, "Structure, Elastic Constants and XRD Spectra of Extended Solids under High Pressure," *MRS Advances* **3**(8), 499-504 (2018). (doi:10.1557/adv.2018.277) 12.2.2

3. Bennion, J.C., I.G. Batyrev, and J.A. Ciezak-Jenkins, "The High-Pressure Characterization of Melt-Castable Energetic Materials: 3,3?-Bis-Oxadiazole-5,5?-Bis-Methylene Dinitrate," *Propellants, Explosives, Pyrotechnics*, (2018). (doi:10.1002/prep.201800215) 12.2.2

4. Cheng, B., F. Zhang, H. Lou, X. Chen, P.K. Liaw, J. Yan, Z. Zeng, Y. Ding, and Q. Zeng, "Pressure-induced phase transition in the AlCoCrFeNi high-entropy alloy," *Scripta Materialia* **161**, 88-92 (2019). (doi:10.1016/j.scriptamat.2018.10.020) 12.2.2

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Appendix 2: Operating Schedules

2017-2 August - December

Aug-17	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	AP	8968	Mao (Yu				IT	M	s.o.			Wenk		8847	AP	7814	9020	Chen			AP	s.o.				DD			AP	M	S/T
0800-1600	JY		Lin) 8702		Godwal		M	M	m/c				SP	AP	PA	JD		HP*		AP	M	Ciezak-J		m/c	DD	m/c	IHR	AP	M	M	S/T
1600-2400					8743		M	S/T			8954			AP				9027		AP	S/T	8531			DD			AP	M	S/T	S/T

Sep-17	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
	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/T	S/T	S/T	H	M	S/T	S/T		Zenh			AP	DD	8968	8847		IT	AP	M	s.o.				8376		AP			9071	
0800-1600	S/T	S/T	S/T	H	M	S/T	m/c		HP*		AP	DD	JY	SP	Shim		AP	M	M	m/c	Soghom.		JL	IHR	AP	m/c	IHR	Li	QW/EFO	
1600-2400	S/T	S/T	S/T	H	S/T	S/T			8980		AP	DD			8225		AP	M	S/T		8668				AP	IHR		HP*	7703	

		User Mtg																	EQ-day												
Oct-17	**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	7703	IT	M	s.o.		9247	Tolbert			AP		DD	Burtch			AP	M	s.o.	9247	QW/EFO	7703	IT	IT	AP		8847		Miyagi			M
0800-1600	SP8847	M	M	m/c	Yue		8381		AP	IHR	DD		9054		AP	M	M	Yue	IHR		IT	IT	IT	m/c	SP			9145		M	M
1600-2400		M	S/T		HP*				AP		DD				AP	M	S/T	HP*			IT	IT	AP							M	S/T

					MK ICOTOM																									
Nov-17	**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	T	W	Th	F	S	Su	M	T	W	Th
0000-0800	s.o.	9247	DD		QW /		AP			Jackson			AP	Sfty	M	s.o.			8732	8376	8968	AP	H	H	H	H	S/T	AP		AP
0800-1600	Yue	DD			Vennari	AP	m/c			8826		AP	Sfty	M	M	m/c	Mao		JL	JY	Gurlo	IHR	H	H	H	H	AP	m/c	Gurlo	IHR
1600-2400	HP*	DD			8337	AP						AP	Sfty	M	S/T		(Reagan)					IT	H	H	H	H	AP			

														MK Out																	
Dec-17	**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	IHR	Monteir			M	AP	s.o.	AP			8376	AP		AP		Zeng			AP	AP		H	H	H	H	H	H	H	H	H	H
0800-1600			o	M	M	AP	Gurlo	Stavrou		JL	AP	IHR	Gurlo	IHR			7839	AP	Gurlo	IHR	DD	H	H	H	H	H	H	H	H	H	H
1600-2400			7680	M	S/T	AP		8127			AP							AP			DD	H	H	H	H	H	H	H	H	H	H

ALS BL 12.2.2 Operating Schedule

2018-1 January - June

Jan-18	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	H	M	M	M	M	M	M	M	M	S/T	S/T	S/T	S/T	S/T	H	S/T	S/T	BLC					M	AP	s.o.					AP	
0800-1600	H	M	M	M	M	M	M	M	M	S/T	S/T	S/T	S/T	S/T	H	S/T	BLC			STOE		M	M	AP			Stoe		AP	Stoe	
1600-2400	H	M	M	M	M	M	M	M	S/T	S/T	S/T	S/T	S/T	S/T	H	S/T	BLC					M	S/T	AP					AP		

Feb-18	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
	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		m/c			8376	M	IT	m/c	IHR			AP	DD	8968	9442	9657			H	M	M	AP	s.o.			8376	AP	m/c
0800-1600	m/c	Ding 8997		JL	M	M	m/c	IHR	8531 Ciezak-J		AP	DD	JY	Mechot	Karun		Mao / Reagan 8732		H	M	M	AP	Stavrou 8127		JL	AP	m/c	IHR
1600-2400	m/c				M	S/T	m/c	IHR			AP	DD							H	M	S/T	AP				AP	m/c	IHR

Mar-18	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	IHR	IHR			IT	M	s.o.					AP	m/c	9540	9657	IHR	DD	8968	8376	M	AP	s.o.	IHR				AP	m/c	IHR	DD	
0800-1600	IHR	Monteiro 9495			M	M			Miyagi 9145		AP	m/c	OT	Karun	IHR	DD	JY	JL	M	M	AP	IHR	Tolbert 8381			AP	m/c	IHR	DD	Wenk 8954	
1600-2400	IHR				M	S/T					AP	m/c			IHR	DD			M	S/T	AP	IHR				AP	m/c	IHR	DD		

Apr-18	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	S	Su	M
0000-0800	8954	8954	M	IT								AP	AP			IHR	M	AP	s.o.	AP	9647		9144	AP			m/c			
0800-1600	8954	M	M			2-bunch					AP	Gurlo	Ciezak-J 9578		IHR	M	M	AP	Gurlo	Mao / Girzis		Zhou	AP	Gurlo		m/c		HP*-Liu 9433		M
1600-2400	8954	M	S/T								AP				IHR	M	S/T	AP					AP			m/c				M

May-18	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	M	IT	AP	9657	8954	9672	AP	m/c	AP	DD				9144	M	AP	s.o.	m/c				AP	IHR	IHR				H	M	M	IT
0800-1600	M	Gurlo	Karun	Wenk	Wenk	AP	m/c	Gurlo	DD	EOB	Shim 8225		Zhou	M	M	AP	m/c		Kavner 9621		AP	IHR	IHR	Wenk 9672		HP* - Zeng 8980		H	M	M	m/c
1600-2400	S/T			8954	9672	AP	m/c		DD	9502				M	S/T	AP	m/c				AP	IHR	IHR					H	M	S/T	m/c

Jun-18	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
	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	m/c	IHR	8968	IHR	Sfty	DD	9071	9453			9144	M	AP	s.o.					AP	m/c	9442	9657			AP	M	IT	m/c	DD	
0800-1600	IHR	JY	IHR	Sfty	DD	Wenk	Guan	Pravica 9421		Zhou	M	M	AP	EOB	HP*-Yan 9408			AP	m/c	Meshot	Karun	Urban 9625		AP	M	M	m/c	DD	Ciezak-J 9379	
1600-2400	IHR		IHR	Sfty	DD	HP*	HP*				M	S/T	AP	9502				AP	m/c					AP	M	S/T	m/c	DD		

Jul-18	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	9379	9144	9657	H	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M
0800-1600	Zhou	Karun	m/c	H	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M
1600-2400			m/c	H	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M

ALS BL 12.2.2 Operating Schedule

Cycle 2018-2: July - December

Aug-18	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	M	M	S/T	S/T	S/T	S/T	S/T	S/T	S/T	S/T	BLC	BLC	BLC	BLC	m/c	m/c	DD	9657	8968	IHR	M	AP	s.o.	9966	DD	Sheng		AP	m/c	m/c	IHR
0800-1600	M	M	S/T	S/T	S/T	S/T	S/T	S/T	IT	BLC	BLC	BLC	BLC	m/c	m/c	DD	Karun	JY	IHR	M	M	AP	JL	DD	HP*		AP	m/c	m/c	IHR	9893
1600-2400	M	S/T	S/T	S/T	S/T	S/T	S/T	S/T	S/T	BLC	BLC	BLC	BLC	m/c	m/c	DD			IHR	M	S/T	AP		DD	9435		AP	m/c	m/c	IHR	

Sep-18	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
0000-0800	Tolbert		H	M	M	IT	ES			AP	m/c	IHR	IHR	9657	HP*			M	AP	s.o.	m/c				AP			Miyagi		
0800-1600	9893		H	M	M	DD 372	Ciezak-J		AP	m/c	IHR	IHR	Karun		Zhang		M	M	AP	m/c		Wenk		AP	Earl					
1600-2400			H	M	S/T		9575		AP	m/c	IHR	IHR			9433		M	S/T	AP	m/c		8954		AP	9502			9145		

Oct-18	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		8968	M	IT	m/c			AP					IT	IT	IT	IT	M	s.o.	9966	9657	Zeng		AP			DD				M	IT
0800-1600	JY	M	M	m/c	Monteiro		AP			Birgeneau		IT	IT	IT	IT	M	M	JL	Karun	HP*		AP	Ciezak-J		DD		Kavner		M	M	m/c
1600-2400		M	S/T	m/c	9495		AP			10036		IT	IT	IT	IT	M	S/T			8980		AP	9379		DD		9621		M	S/T	m/c

Nov-18	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	m/c				AP	9966	9657	IHR	IHR	HP*			M	AP	s.o.							H	H	H	H	IT	M	S/T	m/c	IHR
0800-1600	Monteiro		Yang	AP	JL	Karun	IHR	IHR	Zhang			M	M	AP			2-bunch					H	H	H	H	M	M	m/c	IHR	Gurlo
1600-2400	9495		10058	AP			IHR	IHR	9388			M	S/T	AP								H	H	H	H	M	S/T	m/c	IHR	

Dec-18	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	Gurlo AP		AP	TM	IHR	m/c	m/c	HP*			M	AP	s.o.	9966	m/c			AP	9657	8968		H	H	H	H	H	H	H	H	H	H
0800-1600		AP	DD 365	IHR	m/c	m/c		Li		M	M	AP	JL	m/c	Gurlo AP		AP	Karun	JY	Yang	10058	H	H	H	H	H	H	H	H	H	H
1600-2400		AP		IHR	m/c	m/c		9619		M	S/T	AP		m/c			AP				H	H	H	H	H	H	H	H	H	H	H

Appendix 3. Extended Beamline Feedback/Comments from Users

First Name: XXXXXX
Email Address: XXXXX
Beamline: 12.2.2 (High Pressure)
Start Date:
End Date:
OPERATIONS & EQUIPMENT
Comments:
laser heating was outstanding!

First Name: XXXXXXX
Email Address: XXXXXXX
Beamline: 12.2.2 (High Pressure)
Start Date:
End Date:
OPERATIONS & EQUIPMENT
Comments: The beam dumped only once, for a few hours.
TECHNICAL SUPPORT
Comments: Both Martin and Andrew were extremely helpful. Andrew was able to adjust his schedule to manage safe housing of Be according to lab protocol, so that we had plenty of gaskets ready by beamstart. Martin was rapidly available when we had questions about the laser heating system, despite it being the weekend.

First Name: XXXXXX
Email Address: XXXXXX
Beamline: 12.2.2 (High Pressure)
Start Date:
End Date:

ADMINISTRATIVE SUPPORT & USER COMMUNICATIONS
Comments:
It took several tries to get a working ALS badge, which was somewhat annoying.

GENERAL COMMENTS
Comments:
Would be nice if cafeteria were open on the weekends.

GUEST HOUSE
Comments:
It was unclear that a separate parking permit is needed for the guest house.

First Name: XXXXXX
Email Address: XXXXXX

Beamline: 12.2.2 (High Pressure)
Start Date:
End Date:
OPERATIONS & EQUIPMENT
Comments: computer crushed very often. Need to be replaced.