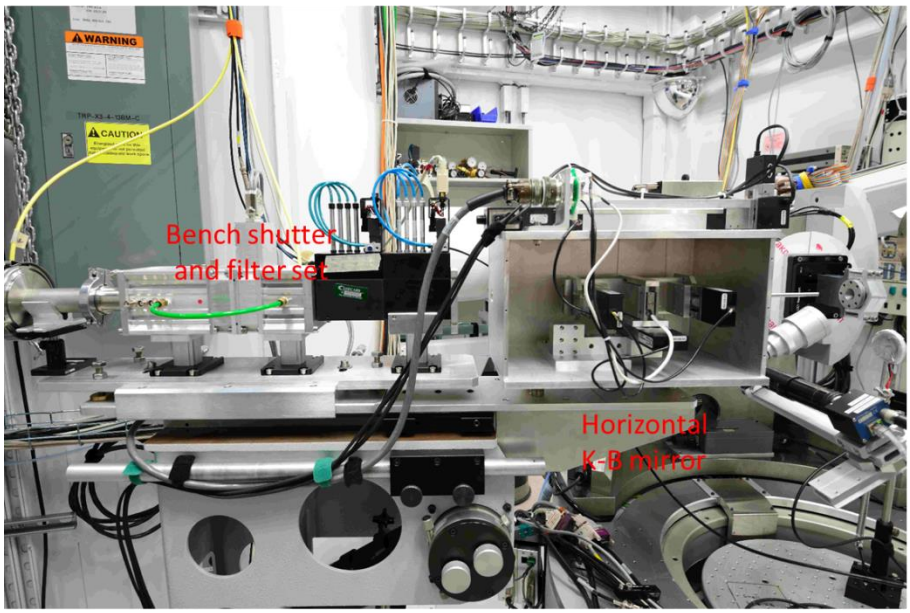
Partnership for Extreme Crystallography (PX^2)
2015 COMPRES Annual Report
November 2014 – October 2015
Prepared by Dongzhou Zhang, Przemyslaw Dera, University of Hawaii at Manoa

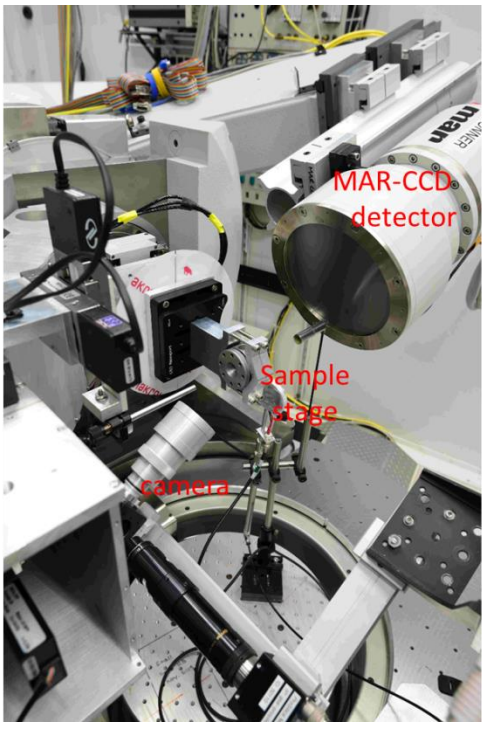
Overview

Partnership for eXtreme Xtallography (PX^2) is providing new capabilities for high-pressure diamond anvil cell research at the GSECARS APS beamline. The PX^2 project is a collaboration between the University of Hawaii and GSECARS, supported by COMPRES and hosted by GSECARS at experimental station 13-BM-C. This beamline provides focused x-rays at two fixed energies: 15 and 28.6 keV and a unique 6-circle heavy duty diffractometer, optimized for a variety of advanced crystallography experiments including interface studies, powder and single crystal structure determination, equation of state studies and thermal diffuse scattering. PX^2 began hosting general users in APS run 2015-1. Currently we support high pressure and temperature experiments using resistively heated diamond anvil cells, and have achieved P-T conditions of 100 GPa and 1000 K during commissioning. We are designing a new compact laser heating system envisioned to extend the temperature range available for diamond anvil cell single crystal experiments. These new capabilities are available to all researchers interested in studying deep earth materials through the APS General User Proposal system.

Experimental instruments

- 50% beamtime, sharing with surface diffraction program of GSECARS
- X-ray energy of 15/28.6 keV, focused to 15×15 micron^2
- Monochromized X-ray with eV bandwidth
- 6-circle kappa geometry diffractometer
- Area detector (MAR165 CCD, Pilatus 100K)
- Resistive heating setup, including power supply, thermal couple temperature reading and water cooling



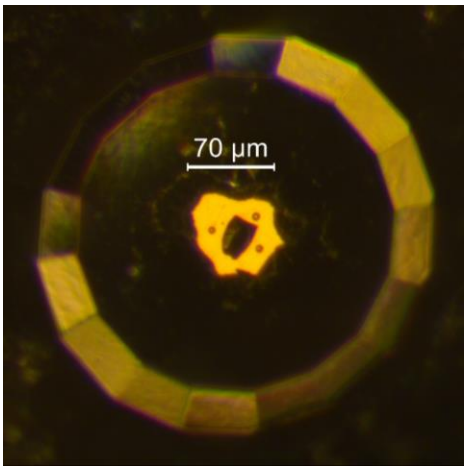


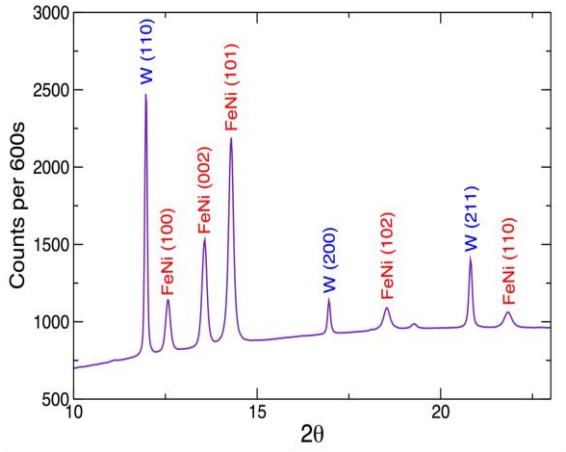
Setup for DAC experiments

Scientific Highlights

- Magnesiowüstite (Mg,Fe)O at high pressure (Greg Finkelstein & Jennifer Jackson, Caltech)

  Magnesiowüstite (Mg,Fe)O is an abundant component in the Earth's lower mantle. Its elasticity and sound velocity data are important to build the seismological model of the Earth. Magnesiowüstite endures a spin-transition under lower mantle conditions, and is a potential candidate to explain the ultra-low velocity zone at Earth's core-mantle boundary. This study measures magnesiowüstite's structural transition and equation of state at high pressures.



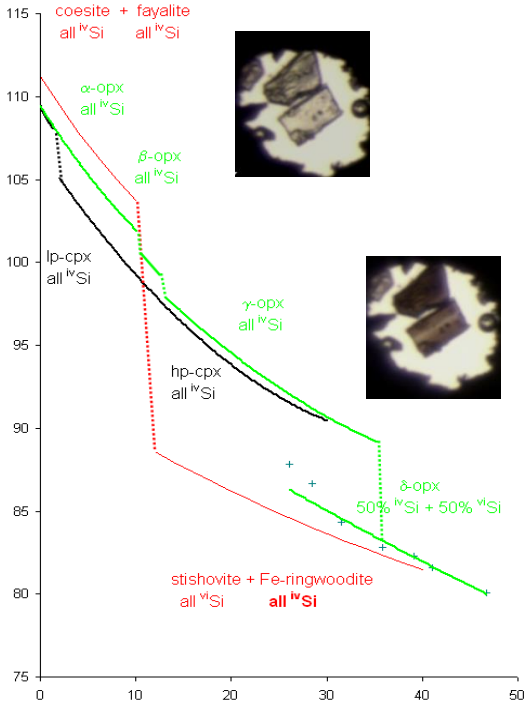


- Diffraction on $Fe_{0.9}Ni_{0.1}$ and W in He loaded cell (Rachel Morrison & Jennifer Jackson, Caltech)

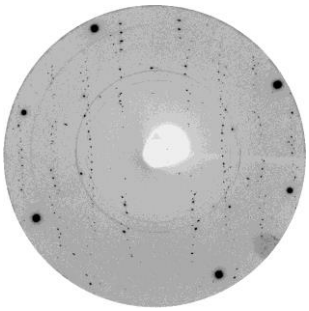
Fe-Ni alloy is believed to be the major component of Earth's core. The phase diagram and sound velocities of Fe-Ni alloy provide important constraints on Earth's internal thermal and chemical structure. This study measures the isothermal equation of state of $Fe_{0.9}Ni_{0.1}$ up to Mbar pressure. He is used as pressure medium to provide hydrostatic environment, and W is used as the pressure marker.

- Structure transitions of mantle silicate ferrosilite (Yi Hu & Przemek Dera, UH Manoa)

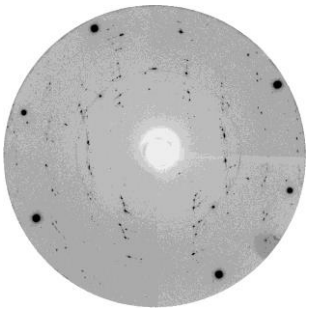
  Large part of the world most significant seismic activity is associated with convergent margins and subduction. Polymorphic phase transitions affect buoyancy relations within the subduction zone and determine the slab's ability to penetrate to the lower mantle. Structural aspects of these polymorphic phase transitions in silicate minerals are studied in diamond anvil cell at the PX^2 facility.



- Thermal stability of ferrosilite at high pressures and its application to subducting slabs (Yi Hu, UH-Manoa)



Pbca, 55 C, 6.2 GPa

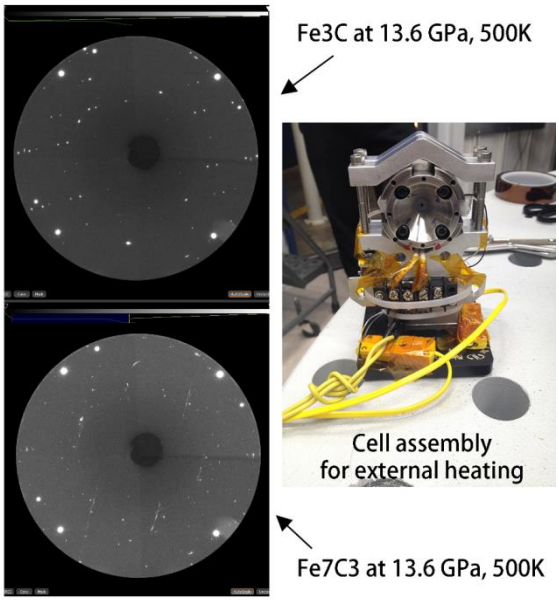


C2/c, 170 C, 8 GPa

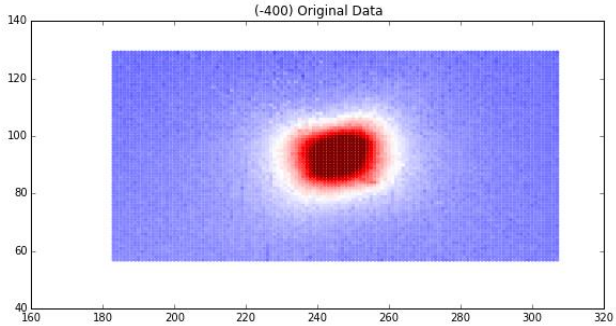
Pyroxene is a group of major minerals in the upper mantle and subducting slabs. Comprehensive knowledge of the phase diagram, structure and thermal equation of state of opx at such conditions is important for understanding subducting process. Ferrosilite is found to transform to a twinned C2/c phase from Pbca phase at ~ 170 C and 8 GPa by single-crystal X-ray diffraction at 13BMC.

- Thermal equation of state of iron carbides by single crystal X-ray diffraction (Xiaojing Lai, Bin Chen, UH-Manoa)

  Accurate knowledge of the phase stability, thermal equation-of-state and sound velocities of iron-carbide phases (particularly Fe_7C_3 and Fe_3C) under or approaching core conditions are required to test the hypothesis of a carbon-rich inner core. The high P-T measurements on structural and elastic properties of the iron carbide candidates for the Earth's inner core can provide us with essential data to evaluate the effects of magnetic and spin transitions and temperature on the density and elastic wave velocities.

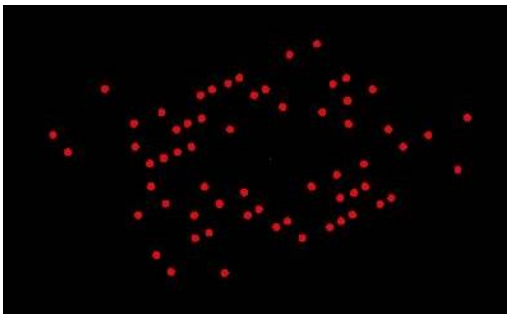


- Thermal diffuse scattering on minerals at high pressure. (Jin Zhang, UH-Manoa/COMPTECH)



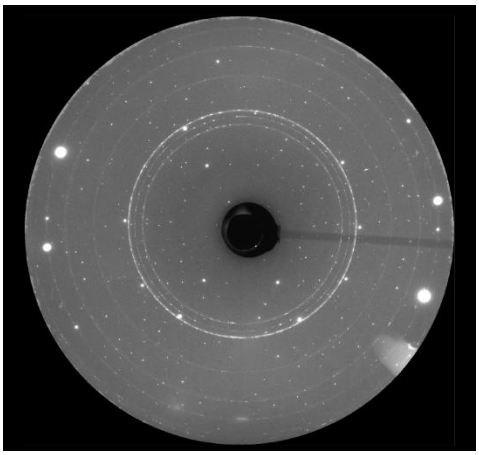
Thermal diffuse scattering is a novel way to measure sample's elastic properties at high pressures. In this study, we collected thermal diffuse scattering data on a variety of materials up to 40 GPa. The figure shows the thermal diffuse scattering signal collected in the vicinity of the Si (-400) peak at ~1.5 GPa.

- High P-T rheology of minerals in a non-hydrostatic environment using single crystal diffraction (Su-Ying Chien, Jiuhua Chen, Dawei Fan, FIU/HPSTAR)



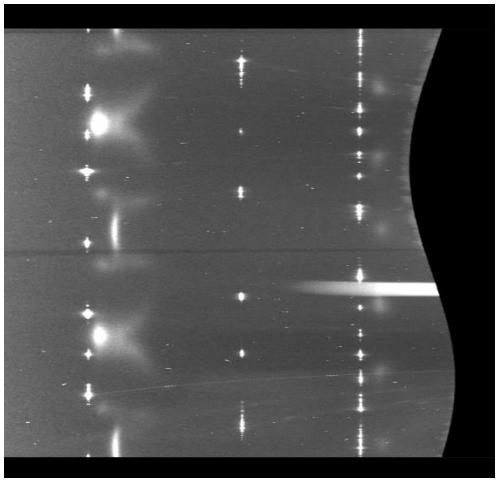
The rheology of mantle minerals provides important information for deep focus earthquakes, mantle convection and dynamics of Earth's interior. This study uses single crystal diffraction to analyze the stress-strain relationship of the sample at high pressures. The strain of the sample is measured by the distortion of the crystal lattice, and the stress is calculated from the diffuse data. The figure shows the lattice of a pyrope sample at 2 GPa.

- Structure stability and phase transition of quasicrystals under high pressure and high temperature (Wenge Yang, CIW)



Quasicrystals have orientational ordering without translation symmetry. From the diffraction, one can get sharp diffraction spots with some forbidden crystalline symmetry, like 5-fold. Recent discovery of nature quasicrystals in a meteorite has pushed the interest of phase stability under high pressure and temperature conditions. This study is aiming to explore the stable quasicrystal $Al_{71}Pd_{21}Mn_8$ synthesized at ambient condition to high pressure and temperature. Angular dispersive x-ray single crystal diffraction at 13-BM-C is employed for the in-situ structure determination. The figure shows the diffraction pattern of the quasicrystal at ~10 GPa.

- Structure of cold-compressed graphite to ultra-high pressure (Liuxiang Yang, CIW)



Carbon is an abundant element with many geological interests. It is involved in many geo- and environment related processes, from climate change to the composition of Earth's core. The origin of diamond, its stability field and its interaction with neighboring Earth material is still under investigation. In this study, single crystal graphite is pressurized to Mbar pressure, and then quenched. A structure in between graphite and diamond is observed in the quenched phase. The figure shows the caked diffraction pattern of the quenched phase.

Personnel

Project PI: Przemyslaw Dera (University of Hawaii at Manoa)
Przemek is the PI of the PX^2 project, but does not receive any salary support.

Beamline scientist: Dongzhou Zhang (University of Hawaii at Manoa)
Dongzhou is the beamline scientist of the PX^2 project. He is responsible for the user support and instrument development at PX^2. Dongzhou has been working in PX^2 since Jan 2015, and is fully supported by COMPRES.

Related personnel:
Mark Rivers (GSECARS, University of Chicago)
Mark is the co-director of GSECARS. He is involved in the beamline upgrade of the PX^2 program

Peter Eng (GSECARS, University of Chicago)
Peter is the beamline scientist of GSECARS in charge of the surface diffraction program of 13BMC. He is involved in the beamline operations and beamline upgrade of the PX^2 program.

Joanne Stubbs (GSECARS, University of Chicago)
Joanne is the beamline scientist of GSECARS in charge of the surface diffraction program of 13BMC. She is involved in the beamline operations and beamline upgrade of the PX^2 program.

Vitali Prakapenka (GSECARS, University of Chicago)
Vitali is the beamline scientist of GSECARS in charge of the diamond anvil cell program. He is involved in the beamline operations and beamline upgrade of the PX^2 program
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Jin Zhang (COMPTECH, University of Hawaii at Manoa)
Jin is in charge of the COMPTECH program of COMPRES. She is involved in the user support of the PX^2 program.

Beamline Operations

PX^2 started operation in the APS run 2015-1. In the runs 2015-1 and 2015-2, about 1/3 of the beamtime was used for commissioning, and was therefore not available for experiments. The total available beamtime in the year of 2015 was 181 shifts (60.33 days). PX^2 is fully funded by COMPRES, and is in close collaboration with GSECARS. With the financial support from COMPRES, we have ordered a new horizontal focusing K-B mirror, a 200 W 1064 nm IR fiber laser for heating, a 1 W 532 nm SPSS laser and a Princeton spectrograph with CCD camera for spectroscopy. All those components will be incorporated into the PX^2 beamline by the end of 2016. GSECARS kindly lend PX^2 several essential instrumentations, including the experimental hutch, the diffractometer, the K-B mirror, the power supplies and digital multimeter for resistive heating setup, the gas loading system and the offline sample preparation lab. Many users of PX^2 also carry out experiments in other GSECARS beamlines, so as to get information about their sample from different aspects.

Number of beamtime proposals received: 22
Number of beamtime proposals granted beamtime: 21
Total number of shifts requested: 232
Total number of shifts granted: 186
Total number of shifts available: 186
Oversubscription rate (= shifts requested / shifts available): 1.25

Number of visits by distinct research groups: 10
Number of unique users, categorized by affiliation
    University: 5
    National Lab/public agency: 4
    Private institution: 1
Number of unique users, categorized by origin:
    USA: 8
    China: 2
Total number of person-visits: 21
Number of undergraduate users: 0
Number of graduate student users: 3
Number of visits funded by each funding agency
    NSF: 10
    DOE: 7
    Foreign: 4

Details of the successful proposals, beamtime allocated, and total usage is provided in the attachment.

Performance Metrics

General User Time for COMPRES: For higher-ranked proposals with beamtime allocated by the facility: 159 shifts was granted to users COMPRES members and foreign affiliates in the year of 2015 (85.4% of total beamtime available), and 121 shifts was granted to users from domestic COMPRES institutions (65.1% of total beamtime available).

Contributing User Time: Allocated for COMPRES users who were not assigned GU time: we don't have any contributing user time in the year of 2015.

Total time for COMPRES users (there will usually be GU and CU COMPRES users): 159 shifts.

Beamline Community Activities

Beamline scientist Dongzhou Zhang received the 2015 MRP Graduate Research Award from AGU.

Beamline Development

1. One major component for high pressure single crystal diffraction is the focusing mirror, because the X-ray position and spot size is critical to the data collection. Single crystal diffraction data with good quality requires both the exact coincidence of the X-ray position and the rotation center of the diffractometer, and an optimal X-ray spot size so that the X-ray fully covers the sample without touching the gasket. Previous horizontal focusing K-B mirror in 13-BMC lacks both accuracy in moving the X-ray position, and a long-enough crystal to focus the X-ray to the optimal spot size without losing flux. With the support from COMPRES, a new horizontal K-B mirror has been purchased for 13-BMC. It features high precision controlling motors and a large high quality silicon crystal. In comparison with previous K-B mirror, the new one has a much finer spatial resolution, better focusing capability, higher X-ray flux as well as improved stability, all of which are beneficial to high quality single crystal diffraction. The new K-B mirror has been commissioned in October, 2015.

2. Proper sample mounting is import for a successful diffraction experiment. In runs 2015-1 and 2015-2, we replaced the out-of-date manual sample observation zooming tube to a state-of-the-art motorized 12X microscope system. Sample alignment can now be carried out remotely with improved precision. Besides microscope, we also added water cooling capability to the DAC holder, which is important to the stability of measurement. Temperatures of more than 1000 K were reached in resistive-heated DACs in our station.

3. The condition of the diffractometer determines the quality of single crystal data collection. The diffractometer in 13-BMC has been used by more than 10 years, so certain wear is unavoidable. Utilizing the shutdown time of the APS, we measured the circles of confusion of the rotation axes of the diffractometer with a laser autocollimator. Some non-coincidence of the rotation axes was observed and corrected.

Planned Activities

1. Ruby fluorescence is one of the most popular methods to determine sample's pressure. Laser heating has been broadly used in the diamond anvil cell community to get in-situ high temperature on the sample. Raman spectroscopy is complementary to diffraction because it provides phonon information of the sample, and is sensitive to crystal structure transition. All the three above techniques are compatible with the current sample observation microscope system, as they share similar optics. We are designing an ultra-compact optical table, which combines the capabilities of viewing microscope, ruby fluorescence, laser heating, temperature reading and Raman spectroscopy. Lasers, illuminators and spectrograph will be coupled through optical fibers, and signals to different detectors will be separated by band-pass filters. The optical table will be designed with compactness, so that it fits into the limited space of the diffractometer without interfering diffraction data collection. Essential parts such as lasers, optical filters and spectrograph has been purchased with the support from COMPRES, and we are planning to finalize the design by the end of 2015, and finish building the optical table by the end of next fiscal year.

2. Resistive heating and temperature readout setup: Resistive-heated diamond anvil cell has been broadly used in contemporary high P-T mineralogy experiments. A remotely-controllable resistive-heating and temperature reading setup has been installed in the experimental station 13-BM-C. It is used by about 1/3 of our users. However, the most important components, the 1000 W power supply and the Keithley digital multimeter, are borrowed from GSECARS, and are shared between GSECARS beamlines. We plan to purchase a set of power supply and digital multimeter in the later part of FY2015, and dedicate them to the 13-BM-C station.

FY 2015 Budget

FY2015 original operating budget form and budget justification for PX^2 are included in table 1.

<u>Personnel</u>

At the end of FY2014 we had $39,974 leftover in direct cost salary funds, because of the later-than-budgeted start of appointment of the PX^2 Beamline Scientist, and different-than-budgeted starting salary level of the new hire. As a consequence, only 6.87 months of salary support for the beamline scientist was requested in FY2015.

PX^2 Beamline Scientist salary and associated fringe benefits have been charged to the project, as budgeted, except for the salary increase. RCUH only allows salary increases in July, therefore the first salary raise will take place in July 2016.

$2,050 in Department of Homeland Security fees was paid for D. Zhang H1 visa processing fees. These charges were approved by the COMPRES President and the NSF Program Director.

In addition to the Beamline Scientist, the machine shop services for manufacturing of beamline components and parts for PX^2 and COMPTECH have been supported through coverage of 0.1 FTE (salary plus fringe) per month of two engineering staff, Mario Williamson and Jonathan Imai, as originally budgeted.

The personnel expenditures in FY2015, projected until November 16, 2015 are:

$30,708	Beamline scientist base salary (5.5 months)
$2,113	Shop engineering staff base salaries (0.1 FTE each)
$32,821	Base salaries total
$13,960	Beamline scientist fringe benefits (5.5 months)
$521	Shop engineering staff fringe benefits (0.1 FTE each)
$19,884	Fringe benefits total

Major equipment

During FY 2015 major commissioning activities related to customization of the 13BMC instrument for the needs of high-pressure experiments took place. All the major equipment components, as outlined in the supplement of 2013 have now been delivered.

The X-ray optics components (new monochromator and Kirkpatrick-Baez horizontal focusing mirror and mirror bender) have been installed, tested and optimized. Sample observation system including motorized platform, motorized zoom microscope and long working distance GeoHeat lens have been installed and aligned.

All major components of the laser spectroscopy system, including Princeton Instruments spectrometer (purchased in FY2014), Laser Quantum Gem 1000mW 532 nm solid state laser, have been delivered, but the commissioning of the spectroscopy system is now planned for 2016 in two stages (first only limited capability ruby fluorescence system, then the full laser-heating system). IPG 200W 1064nm fiber laser was purchased for PX^2 directly from COMPRES Central.

At the end of FY2014 the unspent balance of the 2013 supplement available for capital equipment purchases was $80,406.

Major equipment purchases in FY2015 thus far totaled $20,406 and included:

$6,700	Coastline Optics Si crystal for KB focusing mirror
$10,552	Laser Quantum 1000mW 532nm Gem solid state laser
$295	Newport lens positioner
$462	Thorlabs misc. optical components
$2,397	Newport Agilis mirror mount and controller

A budget plan for the period 11/16/2015-5/30/2016 for the remaining $60K of capital equipment, together with justification, has been submitted for the COMPRES transition to UNM and is included in table 2.

Materials and supplies

In FY2015 no budget for materials and supplies was requested for PX^2. The following major expenditures in this category were made from the leftover of the 2013 supplement and included:

$8,900	Jade Corp - four BX90 DACs, which were not classified as permanent equipment (as originally budgeted), because the price per item was below $5K,
$2,984	EasyLab diamond anvils
$558	Dell and laptop computer for the spectroscopy system
$1,787	Computer, SSD, Hard drives, RAM
$354	Diamond anvil cell tool box
$5,929	Technodiamant standard diamond anvils
$20,512	Total

A balance in the MATERIALS AND SUPPLIES category from the 2013 capital equipment supplement grant and the FY2015 operating budget for the reminder of FY2015 is $19,902.
We also have a balance from the 2013 capital equipment supplement in the amount of $10K in the OTHER (software) category for the reminder of FY2015.

Travel
As originally planned, the PX^2 Beamline scientist participated in the ACA summer school, the COMPRES Annual Meeting, and is scheduled to attend the AGU Fall Meeting (not yet expended). The PI Dera requested support for one trip to APS (not yet expended).

List of travel expenses in FY2015 until November 15, 2015:

$790	ACA crystallography school
$897	COMPRES Annual Meeting, Colorado Springs, CO
$1,687	Total

Other contributions

GSECARS
GSECARS generously contributes significant fraction of time of their staff, Mark Rivers, Peter Eng, Joanne Stubbs, engineering support Mike Proskey, and sector coordinator, Nancy Lazarz to the various activities of this project.
GSECARS donated or lent to the project a number of important and expensive components and electronics, which are used exclusively for the high pressure program. These include e.g. ProSilica camera and MAR165 CCD detector, older KB mirror and bender that were used before the PX^2 horizontal mirror was delivered, etc.
GSECARS covered in full the cost of upgrading the beam transport shielding inside the experimental hutch.

UHM
UHM contributes to the project significant fraction of time of the PI P. Dera. At least 3/4 of the travel expenses associated with the PX^2 activities is covered by UHM. UHM also provides the engineering support services to the project at deeply discounted rate. In 2015 the PI made available to the project at no charge variety of optical components, and several single crystal DACs.

FY 2016 Budget

FY15 operating budget request form for PX^2 is included in table 2.

1. Personnel

The PX^2 Beamline Scientist did not receive a pay increase in 2015. We anticipate a customary inflation-based increase of base salary by 5%, since it will take place after 1.5 years of employment, in June 2016. The projected salary for next year is $70.35K.

Engineering support
Significant commissioning activities will continue at PX^2 through the FY2016, including implementation and optimization of the complex online spectroscopy system. We would like to continue the arrangement with the discounted services of SOEST mechanical engineers, M. Williamson and J. Imai. The cost of this support for the second budget year is calculated based on a discounted monthly 1.0 FTE salary of $ $6,499 for Williamson and $3,500 for Imai, and 1.2 FTE (0.1 FTE per month) months committed for the whole 2016 FY for each of the two engineers.

2. Fringe benefits

Fringe benefits are calculated based on the University of Hawaii at Manoa rate of 42.45%. Fringe benefits for the two engineering staff are calculated at 26.8% (the fringe rate has changed, compared to FY2015).

3. Travel expenses

The PI anticipates requiring travel expense support for the PX^2-related activities at Argonne 1 time a year, with estimated cost of the trip at $2,500.

For the PX^2 Beamline Scientist we request funds to travel to the COMPRES Annual Meeting (estimated cost of each trip is $1,500) and the AGU Annual meeting (estimated cost $2,000).

In the summer 2015 there will be an International High Pressure Crystallography School in Erice, Italy, and we plan for the PX^2 Beamline Scientist to attend this event. Estimated cost of the trip is $3000.

4. Indirect costs

Indirect costs are calculated based on the University of Hawaii approved off-campus rate of 24%.

5. Residual funds

We do not anticipate to have any residual funds at the end of 2015 FY.

Total budget requested: $160,607

Table 1. 2015 PX^2 operation budget for (excluding leftover of capital equipment supplement)

				BUDGET					**YEAR**	2
				Period	06/01/2015-05/31/2016		**FOR NSF USE ONLY**			
ORGANIZATION							PROPOSAL NO.		DURATION (MONTHS)	
University of Hawaii									Proposed	Granted
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR							AWARD NO.		Funds	
Przemyslaw Dera									Granted by NSF	
A. SENIOR PERSONNEL: PI/PD, Co-PI´S, Faculty and Other Senior Assoc						NSF Funded			Funds	
(List each separately with title, A.7. show number in brackets)						Person-months			Requested By	
First Na	M	Last Name	Title			CAL	ACAD	SUMR	Proposer	
1			PI			0	0	0	$0	
(0) TOTAL SENIOR PERSONNEL (1-6)						0	0	0	$0	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						0	0	0	$0	
1. (0) POST DOCTORAL ASSOCIATES						0	0	0	$0	
2. (0) OTHER PROFESSIONALS						0	0	0	$0	
3. (1) OTHER PROFESSIONALS **(PX^2 Beamline Scientist)**						6.87190	0	0	$39,519	
4. (0) GRADUATE STUDENTS									$0	
5. (0) UNDERGRADUATE STUDENTS									$0	
6. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)									$0	
7. (2) OTHER		Engineering support				2.92			$14,603	
8. (0) OTHER										
TOTAL SALARIES AND WAGES (A+B)									$54,122	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS) 45.46%(A) Senior Personnel;									$20,569	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)									$74,692	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000)										
2 BX90 DACs									10,000	
TOTAL EQUIPMENT									$10,000	
E. TRAVEL		1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)							$6,000	
		2. FOREIGN							$0	
F. PARTICIPANT SUPPORT COSTS										
1. STIPENDS				$0						
2. TRAVEL				$0						
3. SUBSISTENCE				$0						
4. OTHER				$0						
($0) TOTAL NUMBER OF PARTICIPANTS									$0	
G. OTHER DIRECT COSTS										
1. MATERIALS AND SUPPLIES									$0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION									$0	
3. CONSULTANT SERVICES									$0	
4. COMPUTERS SERVICES									$0	
5. SUBAWARDS									$0	
6. STIPEND									$0	
7. OTHER									$0	
TOTAL OTHER DIRECT COSTS									$0	
H. TOTAL DIRECT COSTS (A THROUGH G)									$90,692	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)										
Name of indirect cost item				Amount		Rate				
				$80,692		24%	$19,366			
TOTAL INDIRECT COSTS									$19,366	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)									$110,058	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)									$0	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)									$110,058	
M. COST SHARING: PROPOSED LEVEL					AGREED LEVEL IF DIFFERENT $				$0	
PI/PD TYPED NAME & SIGNATURE*					DATE	**FOR NSF USE ONLY**				Initials-ORG
						INDIRECT COST RATE VERIFICATION				
INST. REP. TYPED NAME & SIGNATURE*					DATE	Date Checked		Date Rate of Sheet		
InstRepFullName										
NSF Form 1030 (10/97) ***Supersedes All Previous Editions***						*SIGNATURES REQUIRED ONLY FOR REVISED BUDGET (GPG III.B)				

2015 PX^2 Operation Budget justification

B. Other Personnel

Base salary for full time Beamline Scientist is $67K. A customary inflation-based 3% increase of base salary will be applied on the first day of the month following the anniversary of employment (February 1, 2016). In FY 2015 salary funds are requested for 6.87190 calendar months, with the remainder of the months covered by residual carryover from FY 2014 budget.

Engineering support

During the period of the second budget year of this project significant commissioning activities will continue, including implementation and optimization of the complex online spectroscopy system. COMPTECH will also start actively working on new projects, which will require custom machining of optical and mechanical components. We would like to continue the arrangement with the discounted services of SOEST mechanical engineers, M. Williamson and J. Imai. The cost of this support for the second budget year is calculated based on a discounted monthly 1.0 FTE salary of $ $6,499 for Williamson and $3,500 for Imai, and 2.92 FTE months committed for the whole second year for both of the two engineers.

C. Fringe benefits

Fringe benefits for the scientific staff are calculated based on the University of Hawaii at Manoa rate of 45.46%. Fringe benefits. Fringe benefits for the two engineering staff are calculated at a monthly 1FTE rate of $1,742 for Williamson, and $428 for Imai.

D. Permanent Equipment

All of the PX^2 and COMPTECH projects require diamond anvil cells (DACs) for new experimental method testing and instrument development. We would like to acquire two BX90 DACs, which will be optimal for any high pressure temperature experiments (either resistive heating or laser heating) as well as for multigrain and TDS analysis. A cost of single BX90 DAC is estimated at $5,000.

E. Travel Expenses

The PI anticipates requiring travel expense support for the project activities at Argonne 1 times a year, with estimated cost of each trip at $2,000.

For the PX^2 Beamline Scientist we request funds to travel to the COMPRES Annual Meeting and the AGU Annual meeting. Estimated cost of each of these four trips is $1,500.

We plan that the PX^2 Beamline Scientist will participate in the American Crystallography Association Summer School in 2015. Estimated cost of this expense is $1,000 per person.

I. Indirect costs

Indirect costs are calculated based on the University of Hawaii approved off-campus rate of 24%.

K. Amount of this request

The total request for FY 2015 is $110,058

Table 2. PX^2 budget 11/16/2015-05/31/2016 (all funds)

					BUDGET					**YEAR**	2
					Period	11/16/2015-05/31/2016		**FOR NSF USE ONLY**			
ORGANIZATION							PROPOSAL NO.			DURATION (MONTHS)	
University of Hawaii										Proposed	Granted
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR							AWARD NO.			Funds	
Przemyslaw Dera										Granted by NSF	
A. SENIOR PERSONNEL: PI/PD, Co-PI´S, Faculty and Other Senior Assoc							NSF Funded			Funds	
(List each separately with title, A.7. show number in brackets)							Person-months			Requested By	
First Na	M	Last Name	Title				CAL	ACAD	SUMR	Proposer	
1			PI				0	0	0	$0	
(0)	TOTAL SENIOR PERSONNEL (1-6)						0	0	0	$0	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							0	0	0	$0	
1. (0)	POST DOCTORAL ASSOCIATES						0	0	0	$0	
2. (0)	OTHER PROFESSIONALS						0.0	0	0	$0	
3. (1)	OTHER PROFESSIONALS **(PX^2 Beamline Scientist)**						6.5	0	0	$36,292	
4. (0)	GRADUATE STUDENTS									$0	
5. (0)	UNDERGRADUATE STUDENTS									$0	
6. (0)	SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)									$0	
7. (2)	OTHER	Engineering support					2.6			$13,733	
8. (0)	OTHER										
TOTAL SALARIES AND WAGES (A+B)										$50,024	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS) 45.46%(A) Senior Personnel;										$19,884	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)										$69,909	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000)											
	Optical and optomechanics components for PX^2 laser spectroscopy									$10,000	
	Pi-shaper									$13,000	
	2 Keithley 720 W Resistive heating power supplies									$4,000	
	Keithley digital multimeter for thermocouple readout									$2,000	
	2 SRS signal preamplifiers									$6,000	
	Portable online Raman/ sample visualization setup for COMPTECH PUP projects									$25,000	
TOTAL EQUIPMENT										$60,000	
E. TRAVEL	1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)									$5,000	
	2. FOREIGN									$0	
F. PARTICIPANT SUPPORT COSTS											
1. STIPENDS			$0								
2. TRAVEL			$0								
3. SUBSISTENCE			$0								
4. OTHER			$0								
($0)	TOTAL NUMBER OF PARTICIPANTS									$0	
G. OTHER DIRECT COSTS											
1. MATERIALS AND SUPPLIES										$19,902	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION										$0	
3. CONSULTANT SERVICES										$0	
4. COMPUTERS SERVICES										$0	
5. SUBAWARDS										$0	
6. STIPEND										$0	
7. OTHER										$10,000	
TOTAL OTHER DIRECT COSTS										$29,902	
H. TOTAL DIRECT COSTS (A THROUGH G)										$164,811	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)											
Name of indirect cost item			Amount				Rate				
			$104,811				24%	$25,155			
TOTAL INDIRECT COSTS										$25,155	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)										$189,965	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)										$0	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)										$189,965	
M. COST SHARING: PROPOSED LEVEL					AGREED LEVEL IF DIFFERENT $					$0	
PI/PD TYPED NAME & SIGNATURE*					DATE		**FOR NSF USE ONLY**				Initials-ORG
							INDIRECT COST RATE VERIFICATION				
INST. REP. TYPED NAME & SIGNATURE*					DATE		Date Checked		Date Rate of Sheet		
InstRepFullName											
NSF Form 1030 (10/97) ***Supersedes All Previous Editions***							*SIGNATURES REQUIRED ONLY FOR REVISED BUDGET (GPG III.B)				

PX^2 budget 11/16/2015-05/31/2016 justification for capital equipment

F. Permanent Equipment

The PX^2 project is in final phase of acquitting critical components of the new setup. Majority of these have been funded through the NSF supplement grant in 2013 and the leftover major equipment funds are included in this request.

Optical and optomechanics components for PX^2 laser spectroscopy

We are building a compact optical stage for the PX^2 beamline, on which we plan to install optics for Raman spectroscopy, ruby fluorescence, infrared laser heating and temperature measurement. Raman, ruby fluorescence and temperature reading system will share one spectrometer, which has already been purchased. Some essential optics, such as the high power laser mirrors, beam splitters and optical filters, have been purchased as well. 1064 nm heating laser and 532 nm probing laser are in the process of delivery.

One challenging issue of the proposed optical stage is its size. Our goniometer for single crystal diffraction requires large angular rotations of both the sample stage and the detector, so as to access as many diffraction peaks as possible. If the optical stage is too bulky, the rotation range of the goniometer will be significantly limited, which is not optimal for single crystal diffraction data collection. We need to design an optical stage as compact as possible, while the design cannot be finalized before all the critical components (like the laser) arrive. In addition, the base plate for the stage has to be customized, so that it meets the requirement of minimum spacing. Therefore, we are requesting to reserve $10,000 for the optical and optomechanics components for PX^2 laser spectroscopy.

Pi-shaper

One of the most important parts of the PX^2 system is an innovative compact laser spectroscopy and laser heating setup which consists of Princeton Instruments Cherny-Turner spectrograph with a Peltier cooled CCD detector, green Raman/ruby excitation laser and 200W NIR fiber heating laser. For laser heating application the quality of laser beam profile, including minimal intensity gradients within a large central spot (flat top profile) is essential for reliability of the experiment. This can be achieved by implementing a special compound optics device – Pi-shaper, which has been successfully used at GSECARS 13IDD for several years.

2 Keithley 720 W resistive heating power supplies and 1 Keithley digital multimeter for thermocouple readout

Resistive heating is a technique that is broadly used by the diamond anvil cell community. It provides a stable high temperature environment for the sample, with a gentle temperature gradient. The setup for resistive heating is simple, and it only requires a remote-controlled power supply and a digital multimeter to read the temperature from the thermocouple. In the runs 2015-2 and 2015-3, more than 70% of our users request resistive heating setup, and most of them are from COMPRES member institutions. Currently PX^2 is sharing power supplies and digital multimeter with other GSECARS beamlines. However, with the increasing demands from the users, it is imperative to have a dedicated resistive heating setup in PX^2, so as to eliminate the potential conflicts with other GSECARS beamlines. Some resistive-heated diamond anvil cells, like the Bassett-type hydrothermal DAC, require more than one individually-controlled heaters, so as to adjust the temperature gradient in the sample chamber, so we are proposing to buy two power supplies. One Keithley DMM2700 digital multimeter is enough to read up to 200 thermocouples at the same time, so we only request to buy one digital multimeter.

2 SRS signal preamplifiers

The stability of the X-ray is critical for single crystal diffraction, because a successful single crystal diffraction requires the coincidence of the X-ray focus and the goniometer rotation center over the

exposure time. A feedback system was installed in run 2015-1 to stabilize the vertical position of the X-ray focus. This feedback system is composed of one diagonally divided ion chamber and two SRS preamplifiers, and each preamplifier reads the signal from half of the ion chamber. The offset of the readings from the two preamplifiers gives the relative position of the X-ray beam. The feedback system reads this offset value, and adjust the X-ray focusing mirrors so that the X-ray position is a constant. With the feedback system, the vertical drift of the X-ray beam over the exposure time has been significantly improved. We propose to install the same feedback system to the horizontal direction.

Portable online pressure measurement and sample visualization setup for COMPTECH PUP projects

1. Navitar 12x viewing system with motorized control of focus: $6,000
2. OceanOptics HR2000+ spectrometer, optical fiber, lens and adapter set: $4,500
4. Prosilica GC655 Camera: $1,500
5. Motorized translational stages for moving microscope in and out, focus, and vertical alignment: $10,000
6. Optical and opto-mechanical components including beam splitters, lens and mirrors: $2,000
7. 532nm green laser for ruby fluorescence excitation: $1,000

The portable viewing and pressure measurement setup will be essential for performing high-pressure experiments in non-high-pressure synchrotron beamlines, e.g. sector 34 at APS. The sample chambers used for high-pressure diamond anvil cell (DAC) experiments are in general smaller than 500 um. A long distance working distance lens system with large magnification is necessary for viewing such small sample chamber and positioning the samples. Due to the limited space near sample stage, the viewing system has to be moved out from the X-ray path when collecting data. Navitar 12x viewing system + Prosilica CCD camera + high-precession motorized translational stage setup has been successfully installed in GSECARS for over several years serving this purpose. GE500 532nm green laser and OceanOptics HR2000+ spectrometer will be used for exciting and collecting the fluorescence signal. We could measure ruby fluorescence with X-ray at the same time without removing the sample from sample stage. This whole setup could help high-pressure experiment at any general purpose beamlines, which is important for COMPTECH for exploring possible new techniques for high-pressure mineral physics at different synchrotron beamlines.

Table 3. PX^2 budget request for 2016

BUDGET					YEAR 1
Period 06/01/2016-05/31/2017				FOR NSF USE ONLY	
ORGANIZATION			PROPOSAL NO.	DURATION (MONTHS)	
University of Hawaii				Proposed	Granted
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR			AWARD NO.	Funds	
Przemyslaw Dera				Granted by NSF	

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associate	NSF Funded Person-months			Funds Requested By
(List each separately with title, A.7. show number in brackets)				
First Nam M Last Name Title	CAL	ACAD	SUMR	Proposer
1. PI	0.00	0.00	0.00	0
(0) TOTAL SENIOR PERSONNEL (1-6)	0.00	0.00	0.00	0
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)				
1. (0) POST DOCTORAL ASSOCIATES	0.00	0.00	0.00	0
2. ( ) OTHER PROFESSIONALS	0.00	0.00	0.00	
2. (1) OTHER PROFESSIONALS (PX^2 Beamline Scientist)	12.00	0.00	0.00	70,350
3. (0) GRADUATE STUDENTS				0
4. (0) UNDERGRADUATE STUDENTS				0
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				0
6. (2) OTHER Engineering support	2.40			11,999
7. (0) OTHER				
TOTAL SALARIES AND WAGES (A+B)				82,349
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS) 42.45%(A) Senior Personnel;				38,173
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				120,522
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000)				
TOTAL EQUIPMENT				0
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)				6,000
2. FOREIGN				3,000
F. PARTICIPANT SUPPORT COSTS				
1. STIPENDS $0				
2. TRAVEL $0				
3. SUBSISTENCE $0				
4. OTHER $0				
(0) TOTAL NUMBER OF PARTICIPANTS				0
G. OTHER DIRECT COSTS				
1. MATERIALS AND SUPPLIES				0
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				0
3. CONSULTANT SERVICES				
4. COMPUTERS SERVICES				0
5. SUBAWARDS				0
6. STIPEND				0
7. OTHER				0
TOTAL OTHER DIRECT COSTS				0
H. TOTAL DIRECT COSTS (A THROUGH G)				129,522
I. INDIRECT COSTS (SPECIFY RATE AND BASE)				
Name of indirect cost item: Amount $129,522; Rate 24.0% $31,085				
TOTAL INDIRECT COSTS				31,085
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				160,607
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)				
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				160,607
M. COST SHARING: PROPOSED LEVEL	AGREED LEVEL IF DIFFERENT $			0

PI/PD TYPED NAME & SIGNATURE*	DATE	FOR NSF USE ONLY		Initials-ORG
		INDIRECT COST RATE VERIFICATION		
INST. REP. TYPED NAME & SIGNATURE*	DATE	Date Checked	Date Rate of Sheet	
InstRepFullName				

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