

## **COMPRES Technology Center (COMPTECH)**

2015 COMPRES Annual Report

November 2014 – October 2015

Prepared by Jin S. Zhang and Przemyslaw Dera, University of Hawaii at Manoa

### **Overview**

COMPRES Technology Center (COMPTECH) represents a new model of COMPRES's presence at the Advanced Photon Source, Argonne National Laboratory. It was established to realize the main mission of creating new technical capabilities and preferential access to state-of-the-art facilities at existing beam lines at Advanced Photon Source for the COMPRES community, and help to bring up new and important discoveries in deep Earth interior.

During the past one year, we have been focusing on our main technical development project X-Ray thermal diffuse scattering as a new technique for measuring anisotropic properties under pressure, and several other side projects, including multigrain analysis, universal membrane cap, standard DAC heater and website development. We have made significant progress on all proposed projects, and details are presented in the operations section.

### **Scientific Highlights**

#### **Determination of single-crystal elasticity at high pressure using X-ray thermal diffuse scattering (TDS)**

X-ray thermal diffuse scattering (TDS) has been used to determine elastic properties of solids since 1940s. However, its application in high-pressure mineral physics has not been widely recognized. Sound velocities of Earth materials at relevant high pressure (P) and temperature (T) conditions are essential for interpreting seismic data, which provides by now the most accurate image of the Earth interior. Compared to other techniques used for measuring sound velocities in the high-pressure mineral physics community, for example, Brillouin scattering, stimulated light scattering, inelastic X-ray scattering (IXS), nuclear resonance inelastic X-ray scattering (NRIXS) or MHz/GHz ultrasonics, TDS has several significant advantages and but also some disadvantages. Firstly, it could be used for measuring any single crystals at extreme P-T conditions using diamond anvil cell (DAC), not limited to transparent samples or nuclear resonant isotopes; Secondly, single-crystal elastic properties, not only aggregate elastic properties, could be obtained through TDS, and hence directional dependences of sound velocities are available; Finally, experimental setup for TDS measurement is very easy, no special optical components are needed. However, TDS is much less straightforward in data interpretation, which usually involves micro force constant modeling (Born-von Karman model) to account for interaction between the neighboring atoms.

We developed several alternative experimental strategies of performing TDS experiments at different beamlines (including 13BMC, 13IDC and 34IDE) using different experimental setups (Mar CCD detector, Pilatus detector, flight path, energy scan) with the project PI Dr. Przemyslaw Dera, Sector 34 beamline scientist Dr. Ruqing Xu, GSECARS beamline scientist Dr. Dongzhou Zhang, Dr. Joanne Stubbs and Dr. Peter Eng. We successfully measured TDS up to 40GPa for foresterite and 1.4GPa for Si. J. Zhang also developed Python fitting code, based on continuum elastic wave model, the final fitted single crystal elasticity tensor of Si is identical to what's obtained through the traditional approach using Born-von

Karman model. We also demonstrated the TDS signal to be very sensitive to single crystal elastic anisotropy.

## **Personnel**

Dr. Jin Zhang is the current technology officer, the project and Dr. Przemyslaw Dera from University of Hawaii serves as the PI. The project is now funded by COMPRES through the sub-contract to Hawaii Institute of Geophysics and Planetology. Dr. Jin Zhang joined COMPTECH on November 16<sup>th</sup>, 2014, after the position search process, which was completed in September 2014 (see Attached CV). Dr. Jin Zhang also works closely with the PX<sup>2</sup> beamline scientist Dr. Dongzhou Zhang, who also partially participates in COMPTECH projects.

The Technology Advisory Board (TAB) of COMPTECH oversees and guides the activities of the project. The Board is comprised of synchrotron technology experts, members of the central high-pressure facilities (e.g. HPCAT, GSECARS), managers of the other COMPRES facilities (ALS, NSLS) and mineral physics researchers representing a cross-section of the COMPRES community. Current TAB members include Dr. Quentin Williams (Chair), Dr. Guoyin Shen (HPCAT), Dr. Yanbin Wang (GSECARS), Dr. Lars Ehm (NSLS), Dr. Robert Downs (University of Arizona). Presidents of COMPRES (Dr. Jay Bass (out-going) and Dr. Carl Agee (in-coming)) as well as chairs of the Facilities committee (Dr. Andrew Campbell (out-going) and Dr. Mark Rivers (in-coming)) serve as extra official members of the TAB. TAB meets 3 times per year (January, May and September) through teleconferencing to discuss the activities and progress of the project, as well as to plan future initiatives and actions. In 2015 the TAB also met in person at the COMPRES Annual Meeting in Colorado Springs, CO.

## **Operations and Planned Activities**

There are a total of 6 technical development projects that COMPTECH has been involved in during the reporting period.

### **1. X-ray thermal diffuse scattering (TDS)**

#### **a. Instrumentation:**

The set-up for TDS measurement is identical to regular single-crystal diffraction experiments. We used both Mar CCD and Pilatus detector for the TDS experiments. Although Pilatus detector has significantly higher resolution and lower background than Mar CCD detector, data collected using both detectors provides signal with quality sufficient for TDS data analysis. The flight-path setup, which was originally developed for surface scattering experiments, provides an optimized way to minimize non-sample contribution to the background (Fig. 1).

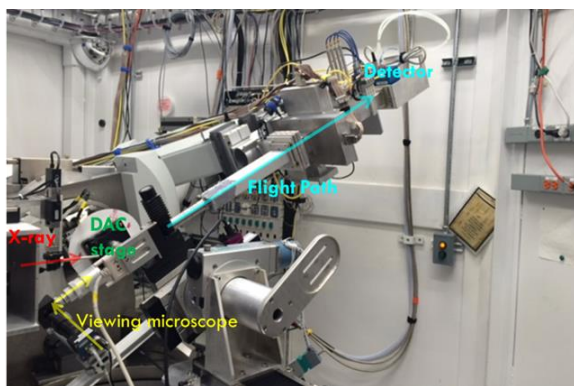


Fig. 1 Flight-path setup in 13BMC for high-pressure TDS measurement

b. Data collection procedure:

We found that the procedure for orientation matrix determination used in surface scattering experiments with flight-path + Pilatus detector setup using SPEC software is quite challenging for TDS measurements in DAC. We were able to develop a set of procedures to find >10 Bragg diffraction peaks for precise determination of sample orientation using SPEC. We are also able to evaluate the crystal quality through rocking curve measurement. In order to eliminate the contributions from other factors that affect to the overall signal shape and intensity (e.g. crystal defects, lattice strain etc.), TDS experiments in general require better crystal quality than single-crystal X-ray diffraction. The signal is measured at slightly off-Bragg-diffraction condition to minimize the contribution from the nearest Bragg peak. We measured the rocking curve for individual Bragg peak to quantitatively determine the crystal quality (Fig. 2). Depending on the incident X-ray beam flux, the collection time varies from 10 minutes (13IDC) to several hours (13BMC).

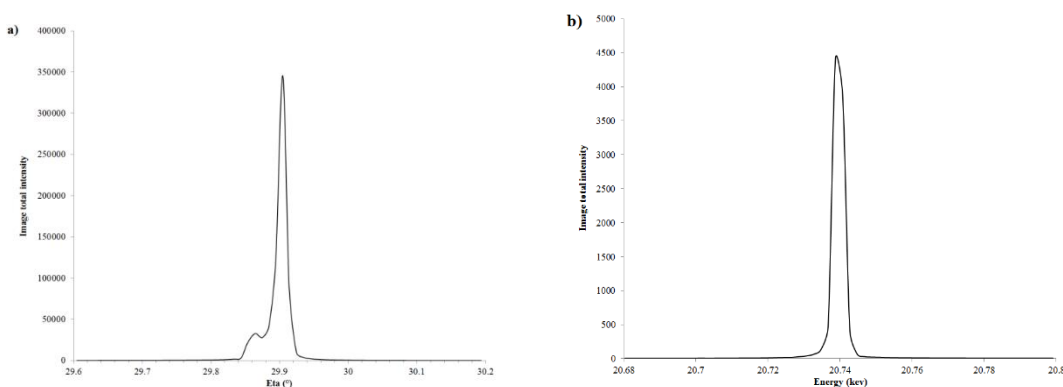


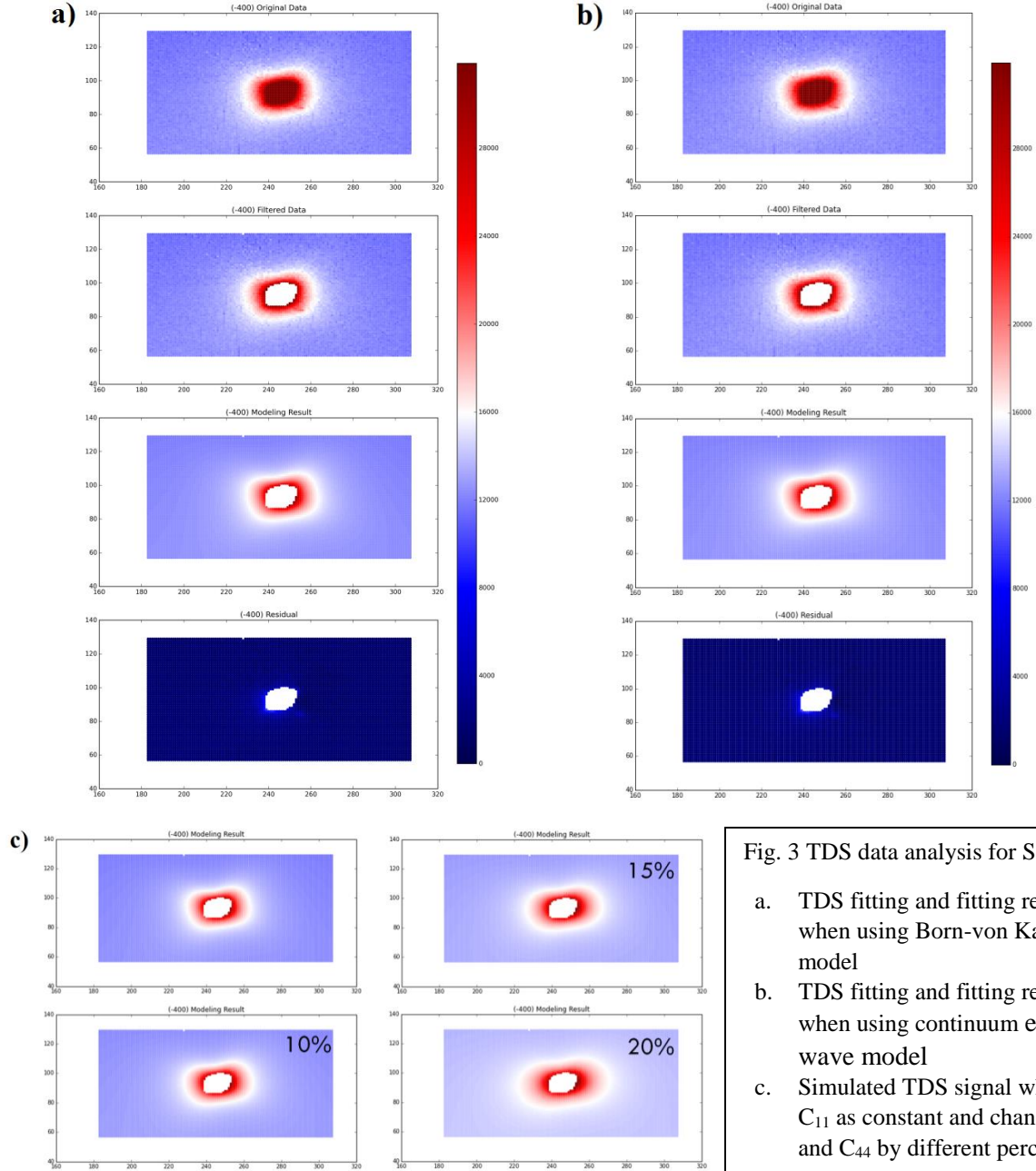
Fig. 2 Rocking curves of forsterite

- a. 13BMC and 13IDC: angular scan approach (6-circle Kappa diffractometer)
- b. 34ID energy scan approach

c. Data analysis:

We have been working on two different data analysis approaches. One is through the traditional Born-von Karman model (micro force-constant model), which needs to be built separately for different crystal structures; the other is based on continuum elastic wave

model under single-phonon scattering assumption, which is universal for different materials with different symmetries. The inversion codes are written in Python; the Born-von Karman model code for Si is written in FORTRAN by our collaborator R. Xu (Fig.3a), and it is callable from Python; the elastic wave model code is written in Python as well (Fig.3b). Detector hkl calibration code was written by P. Dera using IDL, and D. Zhang using Matlab. Through the measurement on single-crystal Si, we proved that these two analysis approaches are equivalent to each other. Simulation also shows that TDS signal shape is very sensitive to single-crystal elasticity (Fig. 3c). We also applied the elastic wave model to foresterite with orthorhombic symmetry, validating the robustness of the inversion code.



d. Future activities (June 2016 - May 2017):

We plan to submit our initial bench-mark high-pressure TDS experimental results for publication in the spring of 2016. We also hope to organize a TDS workshop in summer-fall 2016, and start inviting users to try this new technique from fall-winter 2016.

2. PX<sup>2</sup> instrumentation

COMPTECH researcher J. Zhang participated in the initial instrumentation and pre-alignment of the optical system in 13BMC before the appointment of the PX<sup>2</sup> beamline scientist started in January 2015. J. Zhang also worked on the installation of membrane pressure control system in 13BMC, including ordering of stainless steel tubing, connection of parts and GE Druck PACE5000 pressure controller, and installation of stainless steel tubing inside 13BMC, with the help from GSECARS Mechanical Technician Mike Proskey (Fig. 4). We expect welcoming the COMPRES users utilizing this setup since 2015-3 run.



Fig. 4 Membrane gas tubing in 13BMC

3. Multigrain analysis

COMPTECH researcher J. Zhang prepared sample chambers and participated in the beam time for multigrain analysis in 2015-1 and 2015-2 in HPCAT on laser heating wollastonite and ferrosilite to gain experience on the synthesis process of materials inside of diamond anvil cell.

4. Universal membrane cap

Membrane caps could turn traditional screw-driven DACs into membrane-driven DACs, allowing remote precise pressure control during an experiment. Membrane caps are especially useful for synchrotron experiments. However, current membrane cap designs limit DAC opening to less than 60°. Large DAC opening is essential for high-pressure single-crystal studies, e.g. single-crystal X-ray diffraction, single-crystal Brillouin spectroscopy, etc. In addition, usually each type of DACs requires specific designed membrane cap, therefore, a new design that could fit most DACs is desired, especially at general high-pressure user facilities, e.g. synchrotron beamlines. COMPTECH researcher J. Zhang designed a new type of membrane cap which addresses the above problems. The cap is designed to fit as many different types of DACs as possible, and ensures no loss of diamond anvil cell opening. The membrane cap bulk parts have been received and examined, the membranes are sent back to the machine shop for revision (Fig. 5). We will welcome COMPRES users to use them within the next 2-3 months. Based on the feedback of the users, additional adjustments of the current design will be made by the summer of 2016, and we expect



to have the membrane cap edition 2 machined and tested by spring 2017. All designs will be uploaded onto COMPTECH website for COMPRES users to use.



Fig. 5 Universal membrane cap (bulk parts), 1<sup>st</sup> edition design

## 5. Standard DAC Heaters

Traditional heaters made of Pt wires are very expensive (>\$200/pc), and in general are not useable after 2-3 experiments. The power curve of Pt heater is also not reproducible, varies with pieces. Therefore, cost-effective DAC heaters with standard and stable characteristics are in great demand in high-pressure mineral physics field. The commercial W-Al<sub>2</sub>O<sub>3</sub> metal ceramics heaters are ready-to-use, well-calibrated, reusable, cheap (~\$10) comparing with traditional Pt heaters. They can reach 1000 K within 30 s, temperature is very stable. However their sizes are not suitable for DAC experiments. COMPTECH researcher J. Zhang worked with a vendor of such heaters and developed a modified design of the device, with dimensions that fit DACs. Stacking of two heaters in opposite directions solved the non-uniformity heating of individual heaters. The heaters have also been calibrated both in air and inside DACs (Fig 6). The highest temperature reached in DAC sample chamber when using single piece heater is about 450 K. Higher temperature (500-600K) is expected with the optimized design of double-heaters. Dr. Kurt Leinenweber and Dr. Dan Shim from Arizona State University ordered 20 pcs from COMPTECH for test. We expect to perform more thorough power curve calibration by spring 2016, and distribute to the COMPRES community by summer 2016.

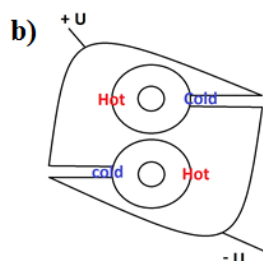
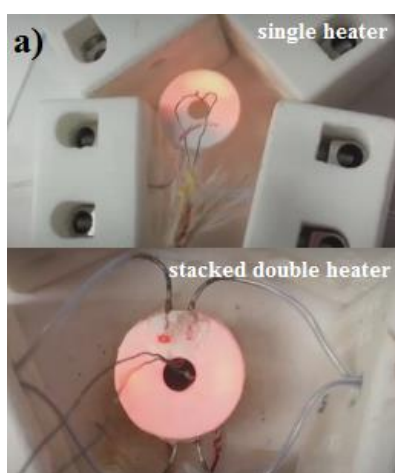
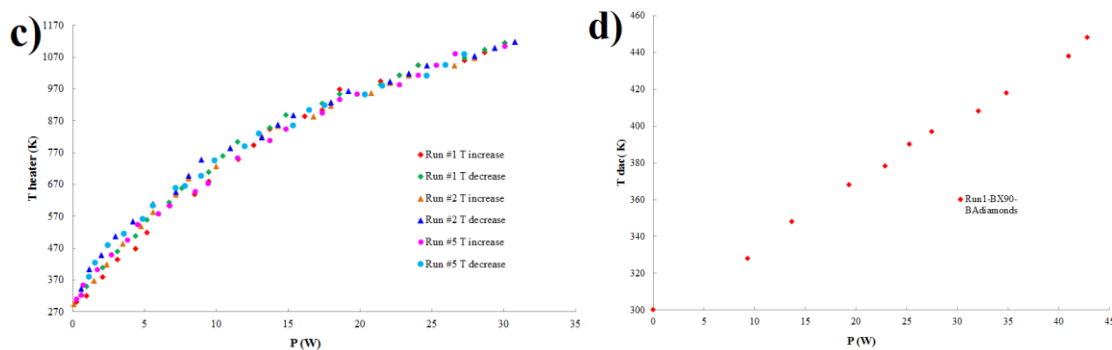


Fig. 6 W-Al<sub>2</sub>O<sub>3</sub> heater

- a. Single heater VS stacked double heater
- b. Stacked heater design
- c. Calibrated power curve of single heater in air
- d. Calibrated power curve of single heater inside DAC



## 6. Website development

The original COMPTECH website was initiated by the former COMPTECH researcher Dr. Bin Chen in 2013. The major component of the old website is the software tools section with JCPDS database integrated. Current COMPTECH researcher J. Zhang rearranged the website, integrating pictures and videos into the website. Major changes include:

- Main home page: include pictures and introduction to the current progress of the main COMPTECH project
- News: Updated with most recent progress of each project;
- Facilities: Added information related to COMPRES supported projects at APS, including 6-BM multi-anvil press beamline; 13BMC PX<sup>2</sup> beamline and GSECARS gas loading system.
- Techniques: It is a new section added for introducing the new progress of the COMPTECH technical development, including TDS, membrane cap and standard DAC Heaters. Instruction files related to each project are also downloadable from the same webpage.
- Tools: Updated with more software tools (e.g. Dioptas), and all software tools are classified under different categories. Software developer's email address and related publications can also be found on the same webpage for user's convenience.
- Advisory Board: It is a new section added for including the information related to technology advisory committee (TAB). All TAB meeting schedules, notes and slides are downloadable from the same webpage.
- Contact: Updated with the current COMPTECH researcher's contact information.

## 7. Preferential access to 34ID-E

One of the primary missions of COMPTECH is to build preferred access to existing non-high-pressure beamlines. 34ID micro-diffraction beamline features some unique advantages: Firstly, the beam size is very small (<500nm), which is ideal for high-pressure experiments with small samples; Secondly, X-ray energy can be adjusted between 7-30 keV, both white beam and monochromatic beam are available. Therefore, high-pressure single-crystal Laue diffraction experiments are possible; finally, both downstream Mar CCD detector and sideways flat panel detectors are

available, and DAC deformation experiments with Be gasket are possible. COMPTECH researcher J. Zhang has performed high-pressure TDS experiments successfully at 34ID. However, 34ID is currently not equipped with any online sample viewing system compatible with DACs, or in-situ pressure measurement system. This currently makes high-pressure experiments at 34ID very inconvenient and difficult. Therefore, COMPTECH planned to collaborate with sector 34 beamline scientists to build up a sample viewing and ruby pressure measurement system for high-pressure experiments. We were able to allocate \$25K in capital equipment funds from the PX<sup>2</sup> supplement budget towards development of simple version of such system with actuation using BIMBA gas cylinder + mechanical stop. Another \$12.5K is needed to properly upgrading the portable system with high-accuracy long-range linear motorized translational stages with step motors for better movement resolution. Request for funds to complete this upgrade has been included in 2016 COMPTECH budget. We will work on commissioning of the optical system during the beam shut down time in 2016: design, order and pre-align the optical components in January, finish the offline alignment in May and finally install it in 34ID in September.

Based on the investments made in this portable system, and the on-going collaboration with the sector 34 scientists on the TDS project, we plan to submit a Partner User Proposal to 34ID-E in 2016.

We will welcome any COMPRES users to use the portable optical system when having beam time at 34ID-E in the future, and we hope that 34ID-E will become a unique and attractive beamline choice for COMPRES users.

## Performance Metrics

### 1. Commissioning experiments

J. Zhang has performed TDS commissioning experiments in the following experimental stations:

13BMC (PX<sup>2</sup> beamline): 2014-3 (15 shifts), 2015-1 (33 shifts), 2015-2 (12 shifts)

13IDC: 2015-2 (6 shifts)

34IDE: 2015-2 (9 shifts), 2015-3 (9 shifts).

J. Zhang has performed multi-grain analysis commissioning experiments in the following experimental stations:

16IDB: 2015-2 (9 shifts)

### 2. COMPRES users

J. Zhang also has helped COMPRES users for PX<sup>2</sup> beam line when PX2 beamline scientist is not present, e.g. Dr. Gang Liu and Liping Kong from HPSync. J. Zhang also discussed possible collaboration opportunities of performing TDS experiments with Dr. Jennifer Jackson, Dr. Bin Chen and HPSync. Dr. Kurt Leinenweber, Dr. Dan Shim from Arizona State University, and Dr. Zhenxian Liu from Carnegie Institution of Washington all asked for the standard metal ceramic heaters offered by COMPTECH for initial test.

### 3. COMPTECH website

The total click counts for the new COMPTECH website during the past 11 months is 1146.



## Community/Broader Impacts

### 4. COMPTECH TAB meeting

In 2015 J. Zhang presented a status report to TAB on COMPTECH projects on January 15th, May 28th and September 23rd. The discussions between COMPTECH personnel and TAB members benefit the development of the COMPTECH project.

### 5. COMPRES annual meeting 2015

J. Zhang presented a status report on COMPTECH projects, mainly focused on TDS experiments. A poster with abstract, experiments setup, data analysis approach and preliminary results has also been presented during the meeting.

### 6. Material Science and Technology 2015 annual meeting

J. Zhang presented her research on utilizing single-crystal X-ray diffraction studying high-pressure phase transitions, introduced and advertised the PX<sup>2</sup> beamline during the meeting.

### 7. IEDA Alliance Kickoff Workshop: mineral physics database

J. Zhang and P. Dera joined the IEDA Alliance Kickoff Workshop at Lamont-Doherty Earth Observatory Columbia University to discuss about future possible opportunities of developing mineral physics data base with IEDA.

### 8. Perspective Users

Several users at 13BMC during 2015-2 run cycle expressed strong interest in trying high-pressure TDS experiments in the near future (e.g. HPSYNC, Xiaojing Lai from University of Hawaii). We also shipped out the first batch of the standard DAC heaters (20 pcs) to Dr. Kurt Leinenweber and Dr. Dan Shim from Arizona State University. Dr. Zhenxian Liu from Carnegie Institution of Washington also asked for 4 pcs for initial test.

### 9. Independent research

COMPTECH researcher J. Zhang finished up writing part of her PhD thesis for developing a CO<sub>2</sub> laser heating Brillouin spectroscopy system for sound velocity measurements at high-pressure high-temperature conditions. J. Zhang also published a paper about a new possible mechanism for generating deep earthquakes with Dr. Lijun Liu from University of Illinois; the majority of the work has been finished when she was a PhD student. She also performed some offline laser heating experiment on hydrous ringwoodite, the quenched products are waiting for analysis during the shutdown time at APS. She is currently working on the high-pressure phase transitions in the faylite system

## Budget status for 2015

The budget form and justification for FY2015 are included in Table 1. Thus far all project expenditures are exactly like planned in the approved budget.

### Personnel

At the end of FY2014 we had \$46,939 leftover in direct cost salary funds, because of the later-than-budgeted start of appointment of the COMPTECH Officer, and different-than-budgeted starting salary

level of the new hire. As a consequence, only 6.12 months of salary support for the COMPTECH Officer was requested in FY2015.

COMPTECH Officer 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.

#### Travel

Thus far the COMPTECH Officer participated in the COMPRES Annual Meeting and presented invited talk at MRS Conference in Ohio. She is also scheduled to participate in the AGU meeting.

\$517	COMPRES Annual meeting
\$1,970	Materials Research Conference in Columbus, OH
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\$2,487	Total

#### Materials and supplies

The expenditure in this category during FY2015 included:

\$4,298	Technodiamant Boehler-Almax diamond anvils
\$1,484	Boehler-Almax WC seats
\$197	Cooksongold, Pt tube
\$362	Si and MgO samples
\$158	Polishing film
\$551	Membrane control tubing
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\$7,050	Total

#### Capital equipment

Two GE Druck pressure gas controllers (\$18,973) were ordered directly through UIUC COMPRES Central and arrived at GSECARS in October

### **Budget Request for FY2016**

#### 1. Personnel

The COMPTECH Officer 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 \$71.4K.

#### 2. Fringe benefits

Fringe benefits are calculated based on the University of Hawaii at Manoa rate of 42.45%.

#### 3. Travel Expenses

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

We request funds to travel to the COMPRES Annual Meeting and the AGU Annual meeting. Estimated cost of COMPRES Annual Meeting is \$1,500, AGU annual meeting is \$2000.

Within development of the TDS technique we would like to conduct an experiment at ESRF, where the technique is already established. We started a collaboration with Prof. Bjorn Winkler and would

like to join his group at ESRF to learn about the details of technique implementation at that facility. Estimated cost of the trip is \$3500.

#### 4.Capital Equipment

Motor upgrade for portable online pressure measurement and sample visualization system

NRT150 for X-Y-Z translation and 1stepper motor controller with 3 channels	\$10,000
desktop/laptop computer for offline motor control:	\$1,500
Additional optical-mechanical components	\$1,000

Materials and Supplies

Diamond anvils and support plates for high pressure experiments	\$2,000
Chemicals, heating wires, gaskets, materials for custom parts machining	\$3,000
Supplies for COMPTECH ID development projects	\$5,000

One mission of COMPTECH is to build preferred access to existing non-high-pressure beamlines. The portable viewing and pressure measurement system is 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  $\mu\text{m}$ . 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. An online ruby pressure system is essential for in-situ pressure determination. We have allocated \$25K in FY2015 capital equipment funds for development of portable optical system with BIMBA gas cylinder + mechanical stop actuation. However, the  $\sim 10 \mu\text{m}$  possitining reproducibility provided by gas cylinder + mechanical stop is not good enough for beamlines with submicron movement precision (e.g. 34IDE) Therefore, we propose to upgrade the current design by replacing the original gas cylinder + mechanical stop design with step motorized long-range precision linear translation stage, which has the resolution of 1  $\mu\text{m}$ . We plan to work on the optical system during the beam shut down time in 2016, design order and pre-align the optical components in January, finish the offline alignment in May and finally install it in 34IDE in September.

One of the major expenses in high-pressure experiments is the cost of diamond anvils ( $\sim \$1\text{K}/\text{piece}$ ). During 2014 COMPTECH acquired a stock of 12 anvils. A budget of \$2K is requested to maintain this stock, perform necessary repairs of damaged anvils, or replace the anvils that are completely broken.

Any DAC experiments will require supplies such as commercially available chemicals as samples or substrates for sample synthesis, solvents, rhenium gaskets for diamond anvil cells, raw materials for machining of custom parts and adapters, etc. A budget of \$3K is requested for these purposes.

COMPTECH projects involve development of portable beam line solutions, and DAC components such as heaters or gas membrane devices for use by COMPRES community. Development and optimization of these devices, requires supplies such as electrical components, thermocouples, stock materials, high temperature cement, etc. A budget of \$5K is requested for these purposes.

#### 5.Indirect costs

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

## 6. Residual funds

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

## Appendices

### 1. CV of the new-hired COMPTECH officer Dr. Jin Zhang

## Jin Zhang

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[University of Hawai'i at Manoa](#)

[Advanced Photon Source](#)

[Argonne National Laboratory](#)

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COMPTECH website: <http://comptech.compres.us/>

Researcher ID (web of science): L-6944-2015

## EDUCATION

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[University of Illinois at Urbana-Champaign](#)

**Ph.D.** in *Mineral Physics*, Aug. 2014      Advisor: Professor Jay D. Bass

[Nanjing University](#), Nanjing, Jiangsu, China

**B.S.** in *Geology*, Jun. 2008      Advisor: Professor Rucheng Wang      GPA: 4.44/5.0      Rank: 1/104

## PROFESSIONAL EXPERIENCE

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**COMPRES Technology Researcher**, *Hawaii Institute of Geophysics and Planetology (HIGP), University of Hawai'i* **Nov. 2014 - present**

**Postdoc Associate**, *Department of Geology, University of Illinois* **Aug. 2014 – Nov. 2014**

**Undergraduate Mentor**, *Department of Geology, University of Illinois* **Fall 2013- Nov. 2014**

- Co-advising undergraduate students: Andrea Vella, Vlad Iordache, and Soojinn Hyung

**Research Assistant**, *Department of Geology, University of Illinois* **Fall 2008-Aug. 2014**

**Teaching Assistant**, *Department of Geology, University of Illinois*

- Lab Instructor of Geology 432: Mineralogy and Mineral Optics **Fall 2010 Fall 2011**

**Assistant Guide**, *Nanjing Museum of Paleontology, Nanjing Institute of Geology and Paleontology*, **2007 – 2008**

**Undergraduate Research Assistant**, *Department of Earth Sciences, Nanjing University*

- Origin of color in red orthoclase, EMPA and IR analysis of granite and pegmatite. **2007–2008**
- Petrology study on Baikal rift basalts, joint field trip with Irkutsk State Technological University. **Aug. – Nov. 2006**
- Geological survey and preliminary modeling of the folds in Phoenix Mountain district, Anhui, China. **Jun. – Sep. 2006**

- Paleontological study on *Globivalvulina* (foraminifera, Car.-Perm.), Shilin, Yunnan, China. **Mar. - May, 2006**

## RESEARCH AREAS

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Structure, composition, and dynamics of Earth's mantle and core

Structure, evolution and dynamic process of lithosphere and subduction slabs

Experimental mineral physics & petrology: phase transition, elasticity, crystallography, spectroscopy

Materials science: Phonon dispersions and phonic crystals

## SKILLS

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### Experimental techniques & Instrumentation:

Synchrotron X-ray: Single-crystal/ powder X-ray diffraction, synchrotron Mossbauer spectroscopy

X-ray thermal diffused scattering (TDS)

Light scattering spectroscopy: Brillouin and Raman spectroscopy, Fourier transform infrared spectroscopy

High-pressure high-temperature techniques: diamond-anvil cells, multi-anvil press, CO<sub>2</sub> Laser heating, resistance heating

Other analysis techniques: Electron probe micro-analyzer (EPMA); scanning electron microscope (SEM)

### Major experimental efforts to date:

- Development of X-ray thermal diffused scattering technique for measuring single-crystal elastic properties of materials;
- Assembly and calibration of a Brillouin scattering system for single-crystal elasticity and diamond cell high-pressure elasticity measurements;
- Design and construction of a Brillouin facility for acoustic dispersion measurements;
- Design and construction of a CO<sub>2</sub> laser-heating system for high-temperature high-pressure Brillouin measurements with the diamond-anvil cell, integrated with Raman spectroscopy and spectro-radiometric temperature measurements.

### Computer Tools:

- Programming skills:
  - Python: development of python code packages for thermal diffused scattering data analysis
  - LabVIEW (CLAD - NI Certified LabVIEW Associate Developer),
  - Other: C/C++, Matlab, html, etc.
- Single crystal X-ray diffraction analysis: GSE\_ADA, GSE\_rsv, Endeavor, etc.
- Spectral analysis and standard software tools: Office, Origin Pro... etc.

## HONORS AND AWARDS

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Harriett Wallace Award, for outstanding woman graduate student: *Department of Geology, University of Illinois* (2014)

R. James Kirkpatrick Award, for graduate student with outstanding research: *Department of Geology, University of Illinois* (2013)



Harriett Wallace Award, for outstanding woman graduate student: *Department of Geology, University of Illinois* (2012)

BP Fellowship Award, for graduate student with outstanding research: *Department of Geology, University of Illinois* (2011-2012)

Department Fellowship, for outstanding entering graduate student: *Department of Geology, University of Illinois* (2008)

10<sup>th</sup> Forum on Sciences and Arts for undergraduate research, discipline of astronomy and geosciences: *Nanjing University* (1<sup>st</sup> place 2007)

5.20 undergraduate research forum of Earth Sciences: *Department of Earth Sciences, Nanjing University* (1<sup>st</sup> place 2006)

People's Scholarship Award: *Department of Earth Sciences, Nanjing University* (1<sup>st</sup> place 2005, 2006; 2<sup>nd</sup> place 2007)

National Fundamental Research Student Award: *Nanjing University* (1<sup>st</sup> place 2005)

#### Invited Talks

**Zhang, J. S.**, Xu, R., Zhang, D., Dera, P., Eng, P. and J. Stubbs, Thermal diffuse scattering as a new technique for determine single crystal elastic properties of materials at high-pressure. AGU Fall Meeting, 2015, San Francisco, CA

**Zhang, J. S.**, P. Dera, B. Reynard, and J. D. Bass. Phase transformations of under extreme pressure temperature conditions: from atoms to Earth. MS&T15 conference, 2015, Columbus, OH

**Zhang, J. S.**, Is upper mantle pyrolitic or not, University of Hawaii, 2015, Honolulu, HI

**Zhang, J. S.**, New high-pressure phase transition in natural orthoenstatite system & sound velocity measurements at simultaneous high pressures and temperatures and variable q by Brillouin spectroscopy with laser heating, University of Illinois, 2014, Urbana, IL

**Zhang, J. S.**, P. Dera, B. Reynard, G. Montagnac, and J. D. Bass Novel high pressure Pbca-P2<sub>1</sub>/c phase transition an overview: Evidence from high pressure high temperature X-ray diffraction and Raman Spectroscopy. IUCr-High Pressure Annual Meeting, 2012, Mito, Japan

**Zhang, J. S.**, P. Dera and J. D. Bass High pressure Single crystal diffraction of Fe-bearing orthoenstatite. Advanced Light Source Annual Meeting, 2011, Berkeley, CA

## **PUBLICATIONS**

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#### Journal Articles (peer reviewed)

1. **Zhang, J. S.** and J. D. Bass, High-pressure single crystal elasticity of San Carlos Orthoenstatite up to 12 GPa and evidence for the pressure-induced Pbca-P2<sub>1</sub>/c phase transition (to be submitted)
2. **Zhang, J. S.** and J. D. Bass, Sound velocities of olivine under simultaneously high P T conditions: is upper mantle pyrolitic... Or not? (to be submitted)
3. **Zhang, J. S.**, Bass, J.D. and G. Zhu (2015), Single-crystal Brillouin spectroscopy with laser-heating and variable q, Rev. Sci. Instrum. 86, 063905. doi: 10.1063/1.4922634
4. Liu, L. and **J. S. Zhang** (2015), Differential contraction of subducted lithosphere layers generates deep earthquake generation, Earth Planet. Sci. Lett. 421, 98. doi:10.1016/j.epsl.2015.03.053
5. **Zhang, J. S.**, Shieh, S., Bass, J.D., Dera, P. and V. Prakapenka (2014), High-pressure single-crystal elasticity study of CO<sub>2</sub> across phase I-III transition, Appl. Phys. Lett. 104, 141901. doi:10.1063/1.4870526

6. Wu, S., Zhu, G., **Zhang, J. S.**, Banerjee, D., Bass, J. D., Ling, C., Yano, K (2014), Anisotropic Lattice Expansion of Three dimensional Colloidal Crystals and Its Impact on Hypersonic Phonon Band Gaps, *Phys. Chem. Chem. Phys.* 16, 8921-8926. doi: 10.1039/C4CP00498A
7. **Zhang, J. S.**, Reynard, B., Montagnac, G. and J. D. Bass (2014), Pressure-induced Pbca-P2<sub>1</sub>/c phase transition of natural orthoenstatite: high temperature effect and its geophysical implications, *Phys. Earth Planet. Int.* 228, 150-159. doi: 10.1016/j.pepi.2013.09.008
8. Zhu, G., Swintek, N.Z., Wu, S., **Zhang, J. S.**, Pan, H., Bass, J. D., Deymier, P. A., Banerjee, D. and K. Yano (2013), Direct observation of phononic dispersion of a three-dimensional solid/solid hypersonic colloidal crystal, *Phys. Rev. B* 88, 144307. doi: 10.1103/PhysRevB.88.144307
9. **Zhang, J. S.**, Reynard, B., Montagnac, G., Wang, R. and J. D. Bass (2013), Pressure-induced Pbca-P2<sub>1</sub>/c phase transition of natural orthoenstatite: Compositional effect and its geophysical implications, *Am. Mineral.* 98, 986-992. doi:10.2138/am.2013.4345
10. **Zhang, J. S.**, P. Dera, and J. D. Bass (2012), A new high-pressure phase transition in natural Fe-bearing orthoenstatite, *Am. Mineral.* 97, 1070–1074. doi:10.2138/am.2012.4072
11. **Zhang, J. S.**, J. D. Bass, T. Taniguchi, A. F. Goncharov, Y.-Y. Chang and S. D. Jacobsen (2011), Elasticity of cubic boron nitride under ambient conditions, *J. Appl. Phys.* 109, 06352. doi:10.1063/1.3561496

#### Book Chapters

- Bass, J.D. and **J. S. Zhang** (2015), Techniques for measuring high P/T elasticity. In Price, G.D., Ed., *Treatise on Geophysics* (2<sup>nd</sup> edition) -Mineral Physics, Elsevier, Amsterdam.

#### Abstracts, Talks and Posters

- Talk (COMPRES Annual Meeting 2015)
- **Zhang, J. S.**, Xu, R., Zhang, D., Dera, P., Eng, P. and J. Stubbs, Determine single crystal elasticity using Thermal Diffused Scattering (TDS), Colorado Springs, Colorado US
- Talk (Japan Geoscience Union Meeting 2015)
- **Zhang, J. S.**, Bass, J.D., Single-crystal Brillouin Spectroscopy with Laser Heating and Variable q: Design, Demonstration and Results on Olivine, Makuhari Messe, Japan
- Talk (AGU Fall Meeting, 2014)
- **Zhang, J. S.**, Bass, J.D., Single-crystal Brillouin Spectroscopy with Laser Heating and Variable q: Design, Demonstration and New Results on Olivine, San Francisco, CA
- Talk (EHPRG 2014)
- **Zhang, J. S.**, Bass, J.D., Single-crystal Laser Heating Brillouin Spectroscopy & Brillouin Spectroscopy with variable q: Design & Demonstration, Lyon, France
- Talk (COMPRES Annual Meeting 2014)
- **Zhang, J. S.**, Bass, J.D., Sound velocity measurements at simultaneous high pressures and temperatures and variable q by Brillouin spectroscopy with laser heating, Stevenson, WA
- Talk (AGU Fall Meeting, 2013)
- **Zhang, J. S.**, Bass, J.D., Sound velocity measurements at simultaneous high pressures and temperatures and variable q by Brillouin spectroscopy with laser heating, San Francisco, CA
- Abstract (the 3<sup>rd</sup> Global-COE International symposium of deep earth mineralogy in conjunction with TANDEM March 2013)

- **Zhang, J. S.**, Bass, J.D., Reynard, B. and P. Dera. Elasticity and structure of mantle pyroxenes. Matsuyama, Japan
- Poster (COMPRES Annual Meeting 2012)
- **Zhang, J. S.**, Reynard, B., Montagnac, G., Wang, R.C. and J. D. Bass Compositional effect to  $\text{Pbca-P2}_1/\text{c}$  high pressure phase transition of orthoenstatite. Williamsburg, VA
- Abstract (AOGS - AGU (WPGM) Joint Assembly 2012 March)
- Bass, J.D., **Zhang, J. S.** and P. Dera. High-Pressure Transition and Sound Velocities of Natural Enstatite. Singapore
- Talk (GSA Annual Meeting 2011)
- **Zhang, J. S.**, P. Dera and J. D. Bass New imagine of Fe-bearing Orthoenstatite phase diagram and its geophysical significance. Minneapolis, MN
- Poster (COMPRES Annual Meeting 2011)
- **Zhang, J. S.**, P. Dera and J. D. Bass High pressure phase transition of orthoenstatite. Williamsburg, VA
- Poster (AGU Fall Meeting, 2010)
- **Zhang, J. S.**, J. D. Bass, T. Taniguchi, and A. F. Goncharov Elastic properties of cubic boron nitride under ambient conditions. San Francisco, CA
- Poster (AGU Fall Meeting, 2009)
- **Zhang, J. S.** and J. D. Bass High pressure elastic properties of natural orthopyroxene up to 18 GPa. San Francisco, CA

## PROFESSIONAL AFFILIATIONS

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American Geophysical Union

Mineralogical Society of America

### 2. Publication list:

Zhang, J. S., Bass, J.D. and G. Zhu (2015), Single-crystal Brillouin spectroscopy with laser-heating and variable  $q$ , Rev. Sci. Instrum. 86, 063905. doi: 10.1063/1.4922634

Liu, L. and J. S. Zhang (2015), Differential contraction of subducted lithosphere layers generates deep earthquake generation, Earth Planet. Sci. Lett. 421, 98. doi:10.1016/j.epsl.2015.03.053

Table 1. COMPTECH budget for FY2015

				BUDGET				YEAR		2	
				Period		06/01/2015-05/31/2016		FOR NSF USE ONLY			
ORGANIZATION								PROPOSAL NO.		DURATION (MONTHS)	
University of Hawaii										Proposed	
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 Name		Last Name		Title		CAL		ACAD		SUMR	
1				PI		0		0		0	
( 0 )		TOTAL SENIOR PERSONNEL (1-6)				0		0		0	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)				0				0		0	
1. ( 0 )		POST DOCTORAL ASSOCIATES				0		0		0	
2. ( 1 )		OTHER PROFESSIONALS (COMPTECH Scientist)				6.12175		0		0	
3. ( 0 )		OTHER PROFESSIONALS				0		0		0	
4. ( 0 )		GRADUATE STUDENTS								0	
5. ( 0 )		UNDERGRADUATE STUDENTS								0	
6. ( 0 )		SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)								0	
7. ( 2 )		OTHER Engineering support				0				0	
8. ( 0 )		OTHER								0	
TOTAL SALARIES AND WAGES (A+B)										\$35,731	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS) 45.46%(A) Senior Personnel										\$16,243	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)										\$51,974	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000)										0	
TOTAL EQUIPMENT										\$0	
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										\$12,500	
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										\$12,500	
H. TOTAL DIRECT COSTS (A THROUGH G)										\$70,474	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)											
Name of indirect cost item		Amount		Rate							
		\$70,474		24%		\$16,914					
TOTAL INDIRECT COSTS										\$16,914	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)										\$87,387	
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)										\$87,387	
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)

# COMPTECH Budget for FY2015

## B. Other Personnel

Base salary for the COMPTECH Technology Officer is \$68K. A customary inflation-based 3% increase of base salary will be applied on the first day of the month following the anniversary of employment (December 1, 2015). In FY 2015 salary funds are requested for 6.12175 calendar months for the COMPTECH Officer, with the remainder of the months covered by residual carryover from FY 2014 budget.

## 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.

## D. Travel Expenses

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

For COMPTECH 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 COMPTECH Scientist will participate in the American Crystallography Association Summer School in 2015. Estimated cost of this expense is \$1,000 per person.

## G. Other Direct Costs

One of the major expenses in high-pressure experiments is the cost of diamond anvils (~\$1K/piece). For the new activities planned in 2015, in particular for TDS analysis we will need to acquire new Boehler-Almax anvils. A budget of \$10,000 is requested to purchase four pairs of anvils and matching backing plates.

\$2,500 is requested for purchase of four legs for an optical table for the offline spectroscopy lab/instrumentation staging area.

## 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 \$87,387.



**Table 2. COMPTECH budget request for FY2016**

BUDGET					YEAR 1	
Period 06/01/2016-05/31/2017					FOR NSF USE ONLY	
ORGANIZATION					PROPOSAL NO.	DURATION (MONTHS)
University of Hawaii						Proposed
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	Funds
(List each separately with title, A.7. show number in brackets)					Person-months	Requested By
First Name	Last Name	Title		CAL	ACAD	SUMR
1. ( )	PI			0.00	0.00	0.00
( )	TOTAL SENIOR PERSONNEL (1-6)			0.00	0.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. ( )	POST DOCTORAL ASSOCIATES			0.00	0.00	0.00
2. ( )	OTHER PROFESSIONALS			0.00	0.00	0.00
2. ( 1 )	OTHER PROFESSIONALS (PX 2 COMPTECH Officer)			12.00	0.00	0.00
3. ( )	GRADUATE STUDENTS					0
4. ( )	UNDERGRADUATE STUDENTS					0
5. ( )	SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)					0
6. ( )	OTHER Engineering support					0
7. ( )	OTHER					
TOTAL SALARIES AND WAGES (A+B)						71,400
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS) 42.45% (A) Senior Personnel						30,309
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)						101,709
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000)						
Motor upgrade for portable online pressure measurement and sample visualization system						12,500
TOTAL EQUIPMENT						12,500
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)						6,000
2. FOREIGN						3,500
F. PARTICIPANT SUPPORT COSTS						
1. STIPENDS		\$0				
2. TRAVEL		\$0				
3. SUBSISTENCE		\$0				
4. OTHER		\$0				
( )	TOTAL NUMBER OF PARTICIPANTS					0
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES						10,000
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						10,000
H. TOTAL DIRECT COSTS (A THROUGH G)						133,709
I. INDIRECT COSTS (SPECIFY RATE AND BASE)						
Name of indirect cost item	Amount	Rate				
	\$121,209	24.0%	\$29,090			
TOTAL INDIRECT COSTS						29,090
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)						162,800
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.i.)						
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)						162,800
M. COST SHARING: PROPOSED LEVEL					AGREED LEVEL IF DIFFERENT \$	0
PI/PD TYPED NAME & SIGNATURE*			DATE	FOR NSF USE ONLY		Initials-ORG
INST. REP. TYPED NAME & SIGNATURE*			DATE	INDIRECT COST RATE VERIFICATION		
InstRepFullName				Date Checked	Date Rate of Sheet	

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\*SIGNATURES REQUIRED ONLY FOR REVISED BUDGET (GPG III.B)