Progress Report

Facility Support: GeoSoilEnviroCARS: A National Resource for Earth, Planetary, Soil and Environmental Science Research at the APS

EAR-1634415 (University of Chicago)

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Project Overview

GeoSoilEnviroCARS (GSECARS) is a national user facility at Sector 13 of the Advanced Photon Source (APS), Argonne National Laboratory. GSECARS provides earth scientists with access to the high-brilliance hard x-rays from this third-generation synchrotron light source. The research conducted on this sector is advancing our knowledge of the composition, structure and properties of earth materials, the processes they control and the processes that produce them. A variety of analytical techniques are being brought to bear on earth science problems: (1) powder, single crystal and interface diffraction; (2) Brillouin scattering; (3) x-ray absorption fine structure (XAFS) spectroscopy; (4) x-ray fluorescence microprobe analysis and microXAFS; (6) microtomography; (7) high-pressure/high-temperature crystallography and spectroscopy using the diamond anvil cell; and (8) high-pressure/high-temperature crystallography using the multi-anvil press.

Impact of the COVID-19 Pandemic

GSECARS operations have been impacted by the COVID-19 pandemic. The following table shows the status of the APS and GSECARS beamlines (4 simultaneously operating stations) during the current award year.

Phase Name	Dates	Beamline activities permitted	Simultaneous on-site staff at GSECARS
Normal Operations	February 15, 2020-March 20, 2020	All	No limit External users permitted
Minimum Safe Operations	March 21, 2020-May 19, 2020	COVID-19 research only	0
Minimum Safe Operations Plus	May 20-May 30, 2020 June 10-June 14, 2020	Non-COVID research, mail-in, remote access Low and medium risk only. No gas-loading.	4 No external users
Shutdown	June 1-9, 2020	None	0
Limited Operations	June 15, 2020-August 13, 2020	Non-COVID research, mail-in, remote access. Gas-loading permitted No radioactive, explosive or biohazard experiments	4 No external users
Shutdown	August 13, 2020-September 13, 2020	Upgrades, maintenance and repairs	8
Limited Operations Plus	September 14, 2020-December 17, 2020	Non-COVID research, mail-in, remote access. Gas-loading permitted No radioactive, explosive or biohazard experiments	8 Limited ANL onsite users possible with special approval
Shutdown	December 18, 2020-January 4, 2021	None	0
Shutdown	January 4-January 18	Upgrades, maintenance and repairs	8
Limited Operations Plus	January 19, 2021-April 21, 2021	Non-COVID research, mail-in, remote access. Gas-loading permitted No radioactive, explosive or biohazard experiments	8 Limited ANL and external onsite users possible with special approval

From March 20 to May 19, 2020 we were not allowed to run any experiments, and no GSECARS staff were allowed on site. In the user runs between May 20 and August 13 we were able to run mail-in samples, and we could have one on-site person per beamline to run the experiments. During this time we installed software to allow users to have remote control of the beamlines. For the final run of the year, from September 15 to December 17 we were able to have 8 on-site staff, or about 50% of the total staff. In this run the remote access was in full operations. Remote users had full control of the beamline workstations, and saw exactly the same screens they would see if they were on-site. Zoom sessions were running as well, so the remote users could communicate with the beamline staff and with each other. In some cases the users could run the night shifts when GSECARS staff were not present, to more fully utilize the available beam time. We also implemented a very convenient mechanism for users to download their data using an interface similar to DropBox.

We have received very positive user feedback about the remote access experience at GSECARS, and we have been able to resume a level of productivity that is not too different from before the pandemic. In fact, it is likely that many users will want to continue in this mode even after on-site access is allowed again, since it saves them the time and expense of travelling to the APS. However, this mode of operation is hard on the beamline staff, since they, rather than the users, must be constantly changing samples, doing sample preparation in the laboratory, etc. This mode of operation is expected to continue at least through the end of the 2021-1 run at the APS on April 21.

13-ID-E Microprobe Technical Developments

Focused Beam Tomography

We continue to develop focused beam tomography methods that make unique use of the spectroscopies available to users at 13-ID-E. We have made significant progress in developing X-ray micro-diffraction (micro-XRD) tomography to determine mineralogy and crystal structure in user samples. In Year 4 we have begun work in developing XAFS tomography approaches that may allow users to directly image the valence states of elements in suitable geologic materials at 1 μm spatial resolution three-dimensionally within un-sectioned materials. Although challenging due to the potential impact of self-absorption, we have been able to demonstrate that this approach is feasible for Fe spectroscopy in basaltic, silicate-glasses through tomographic XAFS analysis of ~200 μm samples of Pele hair glasses from Kilauea. For some materials where sectioning is not feasible, in samples where there is concern that sectioning may alter elemental speciation or for redox sensitive materials in specialized sample containment environments, this will provide new approaches for investigating chemical speciation.

7-element Silicon Drift Diode Detector

We purchased and commissioned a new 7-element silicon drift X-ray fluorescence detector from Mirion/Canberra for the 13-ID-E station. This system upgrades our existing 4-element SDD detectors from Hitachi. This system provides higher throughput due to the larger active area and improved energy resolution for X-ray fluorescence. This has had significant impact in improving detection sensitivity for trace element analysis and spectroscopy, both through improved count rates and by minimizing background overlaps in the energy dispersive spectra.

High Energy Resolution Fluorescence Detector System

We have continued commissioning and expanding our high energy resolution fluorescence detection (HERFD). HERFD X-ray spectroscopy using crystal analyzers will provide our user community improved energy resolution for XAFS measurements. This will provide a unique resource as the only undulator X-ray microprobe in North America able to do both X-ray fluorescence mapping and HERFD on the same sample. In Year 4 we commissioned a new three-crystal HERFD spectroscopy assembly that replaces the single crystal prototype we had in place, tripling the active area for this technique. We are also continuing to finalize the support structures for the analyzer and detector stages that enables our proposed vertical scattering geometry. With support from this grant and additional resources available from NSF-EAR-CH, NASA SSERVI, and DOE Geosciences, we have purchased a suite of additional specific analyzers that will provide users the capability to apply this new HERFD methodology to a broad suite of X-ray emission lines. Using the new technical design, we were able to demonstrate, for example, improved mean detection limits for rare earth elements. Analysis of USGS synthetic silicate glass standard GSA-1G, doped with Eu at a concentration of 5 ppm, provides clearly interpretable spectra using 3 Ge(111) analyzers.

Mounting for Focused-Ion-Beam Samples

We have continued to develop our capability for collecting XAFS spectra from focused ion beam (FIB) sections with additional support from a NASA-LARS grant. We have published the results of our study on alteration effects of the FIB process on XAFS spectra of Ti, Cr, and V, in olivine and pyroxene and have demonstrated the negligible nature of such effects.

Diamond Anvil Cell Technical Developments

Commissioning of a Cryogenic High-Pressure System Integrated with Online Double-Sided Laser Heating and Offline Raman Systems

A large number of high-pressure experiments experience problems resulting from unwanted chemical reactions and element diffusion, caused by a number of factors: carbon diffusion from diamond anvils and reaction with the sample; mass transport during laser heating; sample reaction with pressure medium or/and diamond anvils etc. One of the ways to suppress chemical reactions and diffusion is to keep the diamonds at cryogenic temperatures. There is currently no cryogenic system dedicated for high pressure studies with diamond anvil cell coupled with double-sided laser heating installed at any beamline at APS and available to the user community. In collaboration with DAC Tools we have developed a cryogenic high-pressure system with unique features and it was delivered to GSECARS in March 2020. This system has membrane remote pressure control of the diamond anvil cell and is compatible with the on-line double-sided laser heating system at GSECARS, and off-line Raman systems. We have successfully conducted the first commissioning experiments in the 2020-3 run on an H_2O sample at 23 GPa cooled down to 80K and laser heated to ~5000K with simultaneous collection of high-resolution x-ray diffraction data. We plan to continue commissioning in 2021 and make it available for users in the 2021-3 run.

Portable High-Pressure Controller

To enhance beamline capabilities for remote user operation we have added a portable PACE5000 high-pressure gas controller, for diamond anvil cell compression with membrane canisters. This will be used in the offline Raman lab, including with the new cryostat described above, or at the beamline when a two-membrane system will be used. The two-membrane system provides significant flexibility in pressure paths by allowing multiple compression and decompression cycles with remotely controlled amplitude.

Upgraded Pi-Shaper Optics in the 13-ID-D Station

The pi-shapers for the double-sided laser-heating setup in 13-ID-D have been upgraded. New pi-shapers (AdlOptica Focal-piShaper_1064_Q) and expanders on motorized stages can control the laser heating spot size on sample in the diamond anvil cell remotely in user mode.

EPICS- and Python Software Development for Beamline Control and Data Analysis.

We continued to improve our beamline software packages, adapting them for remote user operation to control the complex systems at the beamlines and supporting labs. We wrote a new user-friendly program for sample alignment with automatic correction of objective distance for various type of windows with different refractive indices. We have added a module to the single crystal collection program that automatically converts files to a format suitable for on-the-fly processing with the commercial CrysAlis software.

New Pilatus CdTe Detector for the 13 BM-D Station.

We have placed an order for the new PILATUS3 1M Hybrid Photon Counting detector with a cadmium telluride (CdTe) sensor. The PILATUS3 CdTe is a large-area, single-photon counting detector, and with CdTe offers highly efficient detection up to 100 keV. Noise-free single-photon counting plus a 20-bit counter and direct conversion allows measuring weak signals next to strong peaks with the best possible signal-to-noise ratio. These properties are very important for collection of weak signals from samples inside diamond anvil cell, large volume press or other high pressure and temperature vessels. The detector will be delivered in the second quarter of 2021 and will be installed in the 13-BM-D station, replacing the outdated and noisy Perkin Elmer flat panel detector. It will advance high-resolution x-ray diffraction capabilities in this station for diamond anvil cell, large volume press and diffraction tomography experiments.

Newport XPS Motor Controller and Scanning Procedures in the 13-ID-D station

We recently purchased a next generation 8 axis, high-performance XPS motion controller capable of controlling a variety of motor types and executing complex coordinated multi-axis motions. It is currently being installed in the 13-ID-D station and optimized control software is being developed.

Multi-anvil Press Technical Developments

Paris-Edinburgh Cell

We continued to develop the Paris-Edinburgh cell (PEC) in 13-ID-C. The PEC incorporates a multi-channel collimator (MCC) for diffracted beam collimation. Double-focusing mirrors were applied to create a small and intense X-ray beam in 13-ID-C. We improved cell assemblies and heating/cooling designs for the PEC expanded experimental conditions to 10 GPa and 2400 K. Structures of a series of silicate liquids, including $MgSiO_3$, $CaSiO_3$, $CaMgSi_2O_6$, and several compositions along the Na_2O-SiO_2 join, have been studied. A new cooling system has been installed to maintain ultrahigh-temperature during those experiments.

In the coming year we will continue to extend the pressure and temperature capabilities in the PE cell to ~15 GPa and >2500 K for liquid structure studies. This requires new anvil and cell assembly designs. A new heater material, boron-doped diamond, is being tested. We will continue to test new anvil geometry for higher pressure experiments. A new motorized pressure generating system is being built, to allow more efficient and precise pressure control.

Ultrasonic velocity measurements on silicate liquids

Ultrasonic velocity measurements on silicate liquids are routinely carried out in the 1000 ton press in 13-ID-D up to 8 GPa and 2500 K. Relaxed sound velocities have been measured on several silicate (diopside, hedenbergite, etc.), as well as carbonate and metallic liquids relevant to the deep Earth. The relaxed velocity data can be directly compared with seismic observations and have been used to tightly constrain equation of state of liquids. Such information, combined with structural data, helps elucidate structure-property relations in silicate liquids.

To complement the above studies on silicate liquids, systematic studies were carried out on the glasses (super-cooled liquids) of the same compositions mentioned above, using a combination of Raman spectroscopy (off-line), x-ray scattering (ID-C, ID-D), and Brillouin spectroscopy (BM-D) in the diamond anvil cell to pressures up to 70 GPa.

In the coming year we plan to develop a triple-stage anvil assembly for using 10 mm sintered diamond cubes in the T-25 module. We will take the advantage of x-transparency of the sintered diamond anvils, to expand capabilities in both ultrasonic velocity and falling-sphere viscosity experiments, which require the ability to view through the entire sample.

Acoustic Emission

Acoustic emission (AE) has been interfaced with two deformation DIA (D-DIA) apparatus in both 13-BM-D and 13-ID-D to investigate failure mechanisms in rocks undergoing phase transformations and metamorphic reactions. A new 22/16 cell assembly (22 mm cubic cell on 16 mm anvil truncations) was developed for studying large rock samples on the order of 10 mm in diameter and 12 mm in length in the larger DDIA. Pressures up to 6 GPa have been reached, with successful AE detection and location. With various broadband transducers covering resonant frequencies from 0.5 MHz to 15 MHz, we have collected several large datasets on size and frequency dependence of AE events. We are collaborating with Prof. Zhongwen Zhan (Caltech) to extract source characteristics of recorded AEs. We are also collaborating with Prof. Lupei Zhu (St. Louis Univ.) in the development of machine-learning algorithms for automatically detecting and locating AE events.

In the coming year we will continue to extend pressure capability in DDIA-30 with AE detection, to test the transformational faulting hypothesis in olivine $(Mg,Fe)_2SiO_4$, for deep focus earthquakes. A 14/10 cell is being tested, which will accommodate samples about 5 mm in diameter and 7 mm in length, with potential pressure capability approaching 15 GPa.

Pink-Beam Tomography

By applying pink-beam tomography to the high-pressure tomography device in 13-BM-D, we succeeded in imaging degassing process in carbonate at high pressure. This technique allows us to track decarbonation-induced mechanical instability in volcanic rocks. We are currently implementing AE detection with the high-pressure tomography technique.

In the coming year we will implement AE detection with the high-pressure tomography apparatus, by modifying anvil designs. This development has the potential of studying seismic tremor precursors of volcanic activities in the laboratory.

Surface and Interface Program Technical Developments

We installed an ultrahigh vacuum system provided by recently retired collaborator Glenn Waychunas from the Lawrence Berkeley National Laboratory. Capabilities include magnetron sputtering and annealing of samples, residual gas analysis, and low energy electron (LEED) diffraction for surface structure characterization. This facility is extremely useful both for preparing and characterizing samples prior to analysis at the APS, as well as for complimentary studies that require UHV conditions not available at the beamline. This year we have added:

- A new digital camera for low-energy electron diffraction (LEED)
- A new digital camera to replace the obsolete Polaroid camera for the X-ray Laue system
- A new chilled water system to support UHV equipment and X-ray tubes

We have performed pilot experiments for in situ electrochemical manipulation of mineral redox during capillary powder diffraction measurements in collaboration with Peter Heaney and Christopher Gorski at Penn State.

We have also worked on refinement of microcrystal surface scattering capabilities, enabling atomic-scale surface structure measurements from crystals as small as 100 um under aqueous solutions (jointly supported by DOE BES Geosciences).

In the coming year we plan the following:

- Installation of a new anaerobic chamber for oxygen-sensitive sample handling and preparation.
- Installation of a new plasma cleaner for removing organics from crystal surfaces as well as optics components.
- Expansion of in situ electrochemistry capabilities for both surface scattering and powder diffraction programs (jointly supported by DOE Geosciences)

- Upgrades to diffractometers in 13-BM-C and 13-ID-C stations, including air-bearing phi stage and hexapod sample manipulation in 13-ID-C (jointly supported by DOE Geosciences)
- Online surface scattering workshop sometime in spring 2021

Microtomography Program Technical Developments

The following were jointly funded with this award and a DOE Geosciences award entitled "Development of X-ray Tomography for Subsurface Rock and Fluid Studies".

Sample Stage System

We have designed and purchased a new sample stage system consisting of an Aerotech HEX300-230HL hexapod and an ABRS250MP air-bearing rotation stage. This stage can carry much taller and heavier apparatus than our existing stage, permitting use of assemblies such as in-situ high-pressure high –temperature triaxial deformation cells. We have completed the design and fabrication of the modifications to the optical table in the 13-BM-D station to accommodate this new stage system. The modified table and stage will be installed for the beginning of the APS 2021-1 run in January 2021.

Tomography Data Collection Software

We took advantage of the COVID shutdown in March-June 2020 to completely rewrite our old IDL tomography data collection software in Python, using a modern object-oriented architecture. The new software is called TomoScan, and it operates as a tomography scan server using the EPICS control sytem. All of the tomography scan parameters are now EPICS Process Variables, so they can be controlled from any EPICS client, including both GUIs and data acquisition scripts written in Python or any other language. These GUI and scripting clients can be run on any computer on the network, and are not constrained to be run within the Python data acquisition server process.

This software was written by the PI, but was done in close collaboration with Francesco De Carlo, who is the group leader of the Imaging Group in the APS X-ray Science Division. Francesco is in charge of 2-BM, 7-BM, and 32-ID tomography beamlines at the APS, and he has now begun to deploy TomoScan on these beamlines. This is excellent because it means we will no longer be doing independent development, and these beamlines will work together to add new features to TomoScan.

Tomography Data Processing Software

We have implemented TomoPy on both the Linux and Windows data processing machines at GSECARS. TomoPy is an open-source Python tomography reconstruction code which has wide support in the community. We intend to replace the existing IDL/tomoRecon reconstruction code used at GSECARS with TomoPy in the future. We have done comparison of the reconstruction quality using both TomoPy and IDL/tomoRecon. We have found that the TomoPy reconstructions are significantly noisier, and the automated entropy based centering significantly poorer than the existing IDL code. This is surprising because they both started with the same underlying Gridrec C code. We are currently trying to understand these differences, and fix TomoPy so that the quality matches IDL. We have also found that the performance of TomoPy is about 33% poorer than IDL on Linux, which is not too bad. However on Windows it is 4.5 times slower. We need to determine the reason for this and fix it, because many of our users prefer Windows for their reconstruction and data processing.

Most sites use TomoPy from the command line. This can be very useful, particularly for scripting many reconstructions to be done on high performance servers. However, many GSECARS users like the current IDL GUI interface, since it is easy to learn and use. We are developing a similar GUI for TomoPy that will be available to our users, and indeed to the entire community.

General User Program

The GSECARS User Program has been in full operation since Fall 1998. Essentially 100% of the available user operations beam time is being allocated through the APS General User Program. The APS Beamtime Allocation Committee allocates 25% of the available time and GSECARS allocates the remaining 75%. Research at GSECARS has resulted in 2,497 publications in the APS database including 256 PhD and Masters theses.

The GSECARS sector continues to be oversubscribed. For 2020 the sector received 546 beam time proposals for a total of 4,244 shifts, which is very similar to the 548 proposals and 4,153 requested shifts in 2019. The oversubscription averaged 2.26 on the insertion device (ID) beamline, and 1.69 on the bending magnet (BM) beamline. Because of COVID-19 the number of experiments run decreased by 29%, from 420 in 2019 to 297 in 2020. This year we do not report any statistics for outside users or user visits, because there were only about 7 weeks of beam time before users were prohibited from coming to the APS on March 20, 2020. Even prior to that date many universities had instituted travel bans. All experiments after March 20 were run with mail-in and remote access. GSECARS has seen a much smaller drop in the number of experiments run than other APS beamlines, and COMPRES beamlines at other facilities, because we were able to quickly and efficiently switch to a remote access mode.

Productivity Summary	2020-1	2020-2	2020-3	2020
ID Experiments	59	49	69	177
BM Experiments	38	41	41	120
Total Experiments	97	90	110	297
Proposals Received	199	194	153	546
Shifts Requested	1509	1503	1232	4244
ID Oversubscription Rate	2.08	2.62	2.07	2.26
BM Oversubscription Rate	1.77	2.02	1.28	1.69
Outside Users (unique)	na	na	na	
User Visits	na	na	na	
Publications				170

GSECARS staff work with prospective users to help them submit beam time proposals, to prepare samples before they arrive, to collect their data, and to analyze the data and prepare it for publication after they leave the facility. Publications resulting from work at GSECARS frequently include one or more GSECARS beamline scientists as co-authors.

Facility statistics

The APS User Office provided us with a spreadsheet listing every experiment run in 2020 at GSECARS. This information is collected by the APS in the Experiment Safety Approval Form (ESAF). This spreadsheet has the following information for each experiment

1. APS Experiment No.
2. Experiment Safety Approval Number
3. Proposal Title
4. APS Proposal Id
5. First Name
6. Last Name
7. APS Badge No
8. Email
9. Institution
10. User Type
11. Employment Level (Graduate student, post-doc, employee)
12. Experiment Start Date
13. Experiment End Date
14. Subject 1 (Earth science, material science, chemistry, physics, etc.)
15. Subject 2 (Earth science, material science, chemistry, physics, etc.)
16. Subject 3 (Earth science, material science, chemistry, physics, etc.)
17. Funding 1 (First funding agency)
18. Funding 2 (Second funding agency)

We added columns for number of shifts allocated plus additional sheets where were entered information that the APS does not collect.

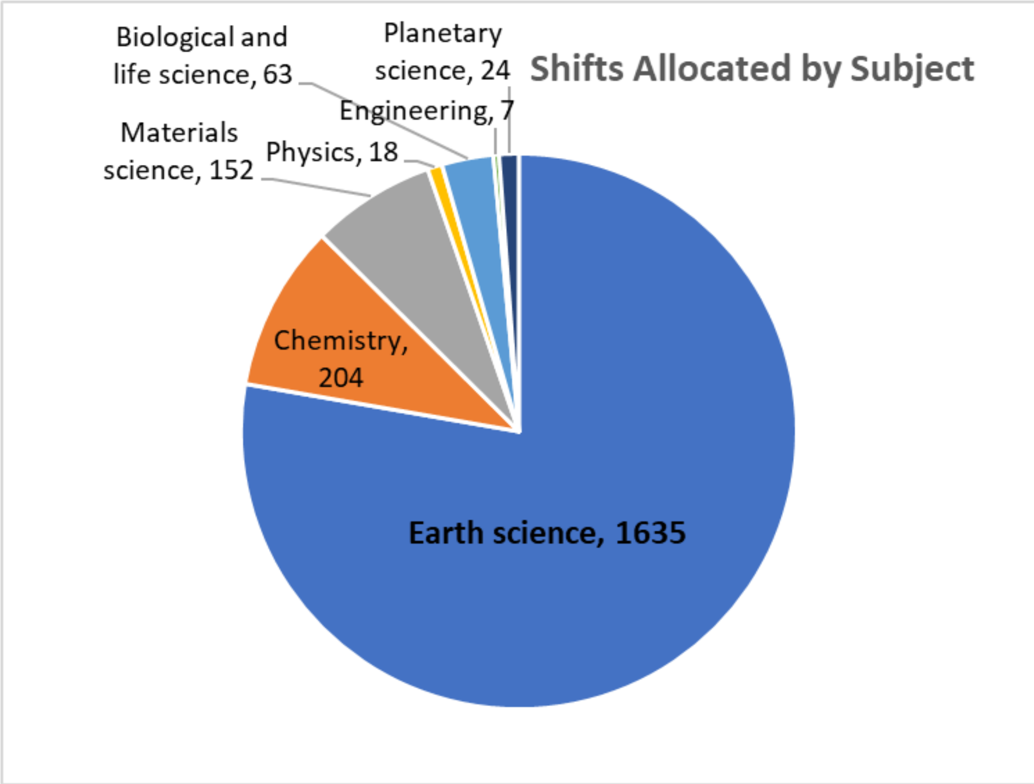
1. NSF Program (EAR, CHE, DMR, etc.)
2. EAR Subprogram (Geophysics, Petrology and Geochemistry, etc.)
3. NSF Grant Number

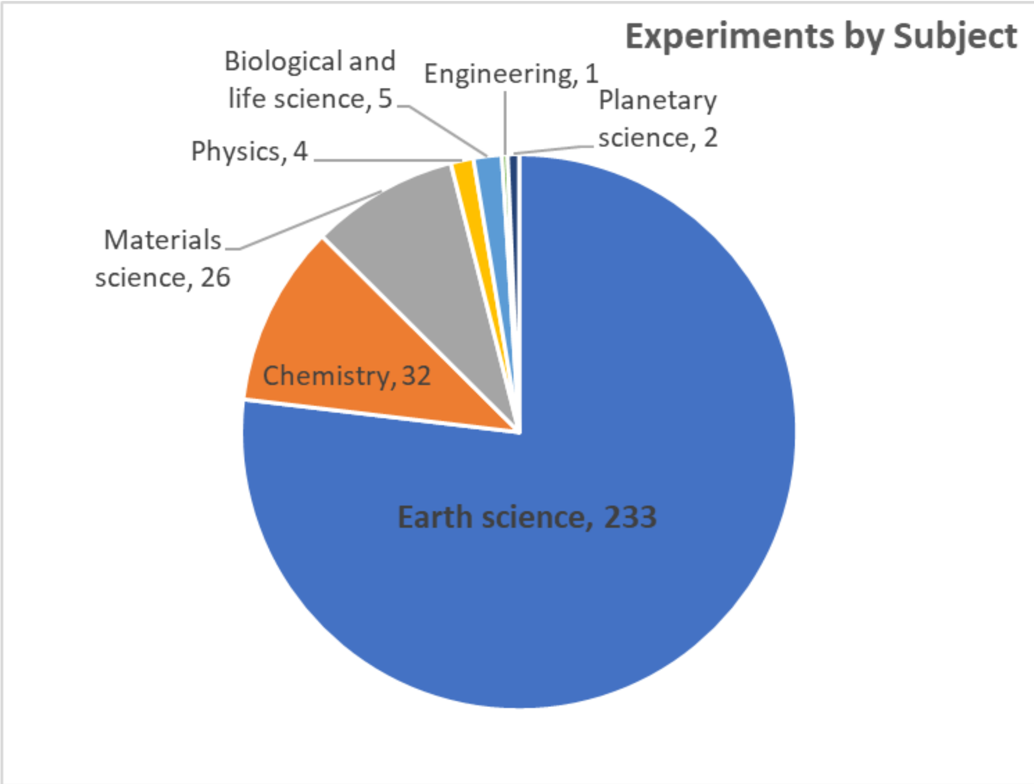
Because there are so many experiments and so much information per experiment it is not feasible to include the text of the spreadsheet in this document. Rather we are providing the spreadsheet itself to NSF, and the following summary table and pie charts in this document.

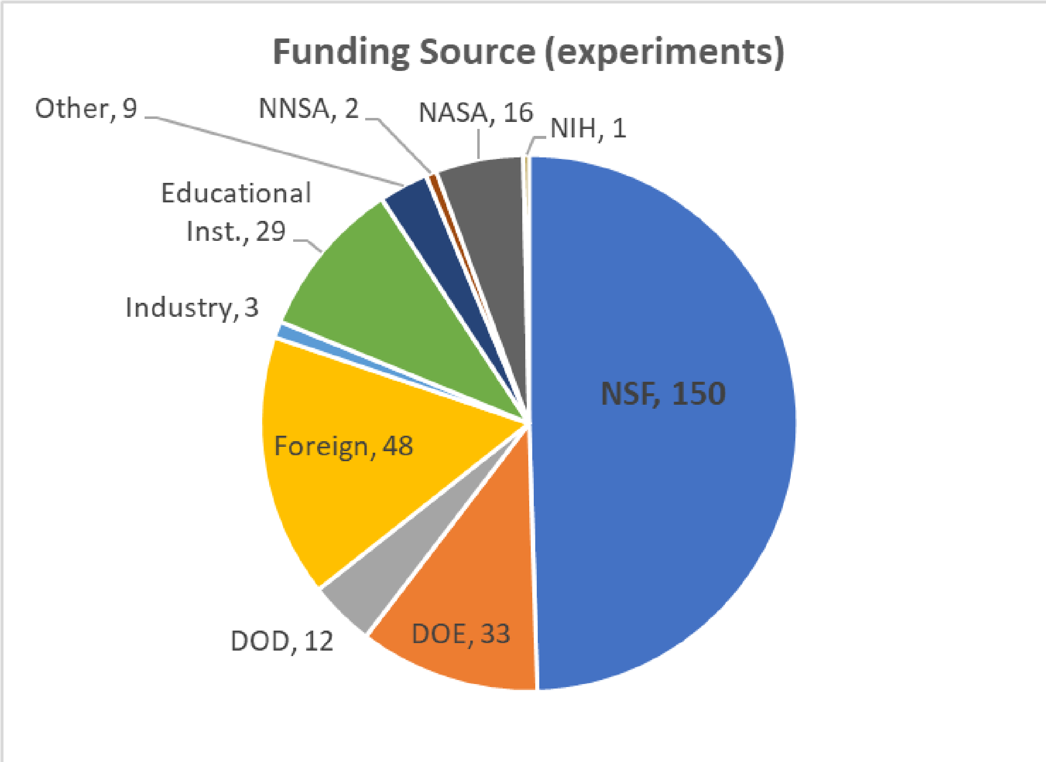
Calendar Year 2020		13BMC	13BMD	13IDC	13IDD	13IDE		Total	Percent
Shifts Allocated (subjects)	Earth science	270	447	75	432	411		1635	77.7%
	Chemistry	75	21	17	37	54		204	9.7%
	Materials science	111	18	0	23	0		152	7.2%
	Physics	15	0	0	3	0		18	0.9%
	Biological and life science	0	6	9	30	18		63	3.0%
	Engineering	0	0	0	7	0		7	0.3%
	Planetary science	0	0	0	0	24		24	1.1%
	Total shifts							2103	
Experiments (subjects)	Earth science	34	53	7	95	44		233	76.9%
	Chemistry	7	4	2	13	6		32	10.6%
	Materials science	15	2	0	9	0		26	8.6%
	Physics	3	0	0	1	0		4	1.3%
	Biological and life science	0	1	1	1	2		5	1.7%
	Engineering	0	0	0	1	0		1	0.3%
	Planetary science	0	0	0	0	2		2	0.7%
	Total experiments							303	
Funding Source (expts)	NSF	20	38	3	65	24		150	49.5%
	DOE	10	3	6	10	4		33	10.9%
	DOD	3	3	0	6	0		12	4.0%
	Foreign	15	7	0	21	5		48	15.8%
	Industry	0	3	0	0	0		3	1.0%
	Educational Inst.	8	5	0	10	6		29	9.6%
	Other	1	0	1	3	4		9	3.0%
	NNSA	0	0	0	2	0		2	0.7%
	NASA	2	0	0	3	11		16	5.3%
	NIH	0	1	0	0	0		1	0.3%
	Total sources							303	
NSF Division (expts)	EAR	8	29	2	44	16		99	90.0%
	DMR	1	2	0	4	0		7	6.4%
	CHE	0	0	0	0	1		1	0.9%
	MG&G	0	0	0	0	1		1	0.9%
	GRFP	0	0	0	0	1		1	0.9%
	DEB	0	1	0	0	0		1	0.9%
	Total NSF experiments							110	
EAR Program (expts)	IF	5	10	0	17	8		40	40.4%
	Geophysics	3	11	2	13	0		29	29.3%
	Petrology & Geochemistry	0	0	0	6	6		12	12.1%
	CSEDI	0	6	0	7	2		15	15.2%
	FRES	0	2	0	1	0		3	3.0%
	Total reported EAR experiments							99	

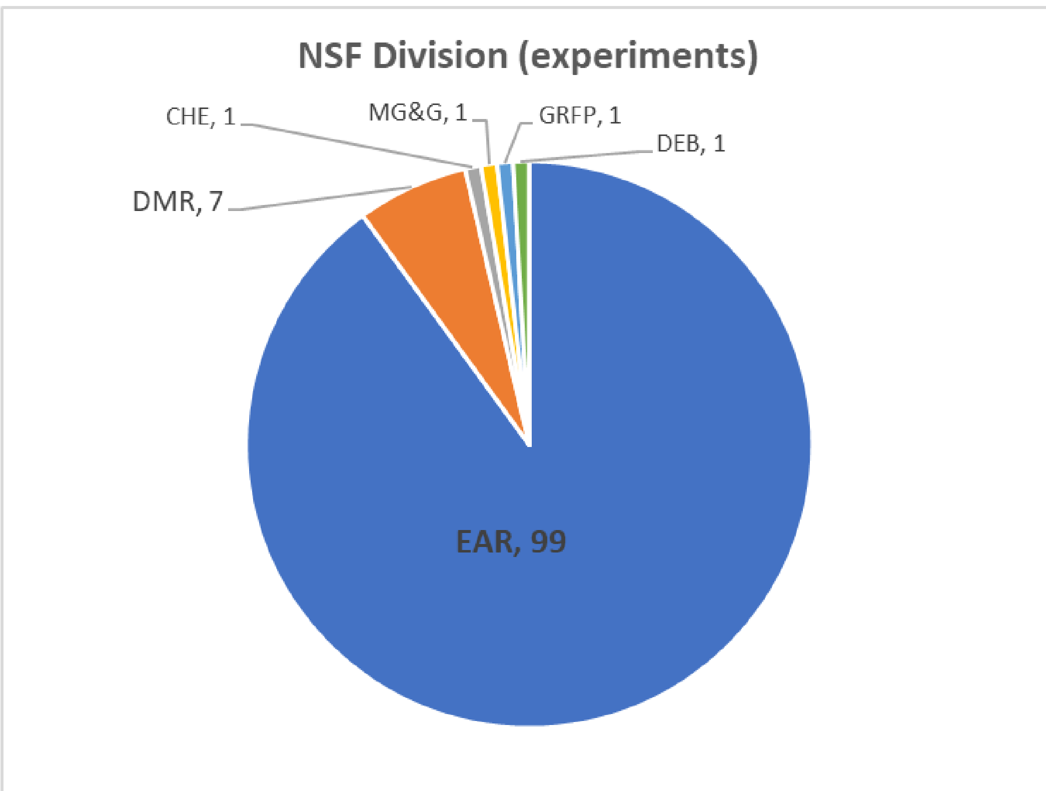
Summary of 2020 user statistics:

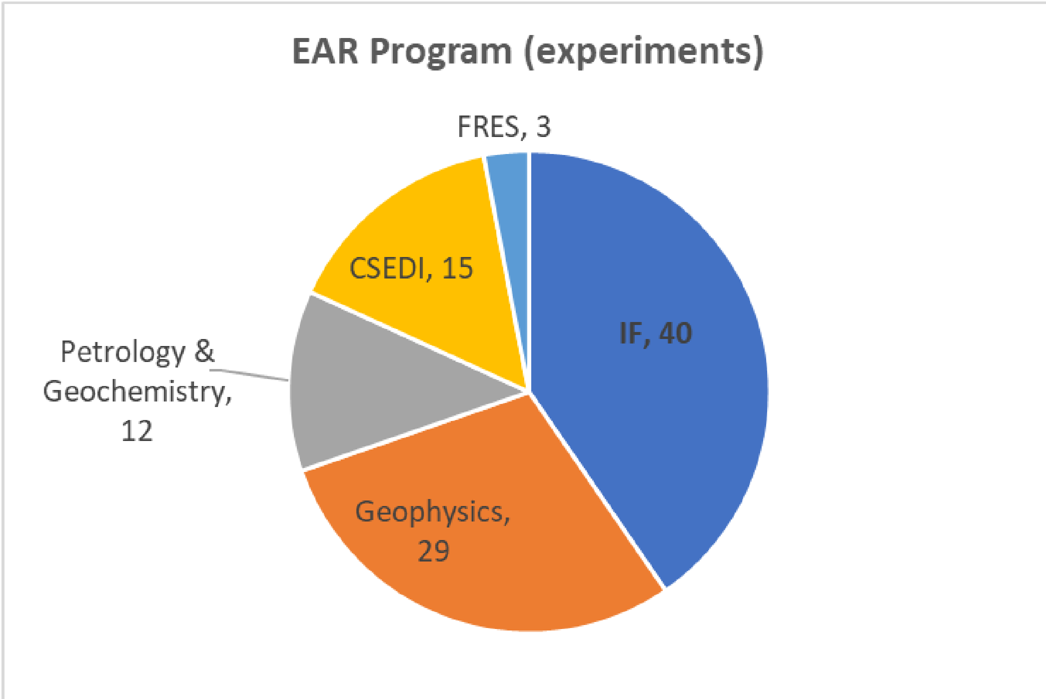
- 77% of the experiments were earth science, both by shifts and experiments.
- There were 303 experiments and we identified main funding sources for all of them.
- 150 experiments were NSF supported (50%)
- We could identify the NSF programs for 110 of the 150 NSF experiments (73%)
- 90% of the 110 NSF experiments were EAR
- We could identify the EAR subprograms for all 99 of the reported EAR experiments
- Some of the 40 NSF experiments with unidentified programs are probably also EAR
- The fraction of IF supported experiments (40.4%) is higher this year than in 2019 (18%) because a larger number of experiments were in-house research by GSECARS scientists, due to the restrictions on user access.


Shifts Allocated by Subject
Biological and life science, 63
Planetary science, 24
Engineering, 7
Materials science, 152
Physics, 18
Chemistry, 204
Earth science, 1635


Experiments by Subject
Biological and life science, 5
Engineering, 1
Planetary science, 2
Physics, 4
Materials science, 26
Chemistry, 32
Earth science, 233


Funding Source (experiments)
Other, 9
NNSA, 2
NASA, 16
NIH, 1
Educational Inst., 29
Industry, 3
NSF, 150
Foreign, 48
DOD, 12
DOE, 33


NSF Division (experiments)
CHE, 1
MG&G, 1
GRFP, 1
DEB, 1
DMR, 7
EAR, 99


EAR Program (experiments)
FRES, 3
CSEDI, 15
IF, 40
Petrology & Geochemistry, 12
Geophysics, 29

Outreach/Expansion Initiatives

GeoSoilEnviroCARS operates as a national research resource for the entire earth, planetary, soil and environmental science communities. GSECARS uses a team approach, where lead individuals (scientists, engineers and technicians) from GSECARS work together with instrument companies and machine shops to design and build the complex array of components that go into a synchrotron station. During this process, we are able to welcome students at all levels— high school, undergraduate, graduate and post graduate— into our laboratory giving them the opportunity to learn about X-ray science and instrumentation as well as to be involved in hands-on activities in which they can experiment at building and testing instruments.

The proposal-based beam time allocation system facilitates the use of this technology by experts and novices alike. Training provided by the experienced GSECARS staff results in direct knowledge transfer to advance the quality of the nation's research infrastructure and to enhance the educational experience of students. Students trained under this program come from educational institutions across the nation and around the world, including the participation of underrepresented groups.

The GSECARS outreach activities are highlighted on our Web site

This year this included:

- Mark Rivers ran a virtual hands-on tutorial on computed microtomography on October 29-30 attended by over 70 people.
- Yanbin Wang, Mark Rivers, and others are organizing an In-situ Studies of Rock Deformation Science Workshop on January 19, 20, and 22.
- Tony Lanzirotti and Mark Rivers hosted a virtual tour for ANL Summer Interns on August 7.
- Matt Newville presented a talk at the ANL high school camp, "Coding for Science".
- Joanne Stubbs worked with eighth graders from local schools in Argonne's Introduce a Girl to Engineering Day on February 7.
- GSECARS hosted high school students from Glenbard East High School. The students ran an experiment at 13 IDE on February 13.

GSECARS also develops numerous hardware designs that are used at many facilities around the world. These include x-ray focusing mirrors, monochromators, and the gas loading system. GSECARS also develops advanced software that is required for our needs, but also benefits the larger scientific community, including many DOE and NSF accelerator facilities. Rivers has collaborated with other groups at the APS in the development of EPICS, a control and data acquisition system for accelerators and beamlines.

In Year 5 we plan to continue these activities.

Management

GSECARS is part of the Center for Advanced Radiation Sources (CARS) at the University of Chicago. Mark Rivers, the PI of this award, is the Executive Director of CARS. CARS operates sectors 13, 14, and 15 at the APS. GSECARS management consists of two Project Managers: (Mark Rivers and Stephen Sutton), and six Technical Groups organized around the six principal techniques in the sector. Each of these groups has a senior GSECARS staff member as a leader as shown below:

- Diamond Anvil Cell (Vitali Prakapenka, Research Professor)
- Large-Volume Press (Yanbin Wang, Research Professor)
- Microtomography (Mark Rivers, Research Professor)
- X-ray Absorption Fine Structure Spectroscopy (Matt Newville, Research Professor)
- X-ray Diffraction and Scattering (Peter Eng, Research Professor)
- X-ray Fluorescence Microprobe (Stephen Sutton, Research Professor)

These individuals have the responsibility to lead the development of science, instrumentation and user community in their particular area. In addition, the leaders work closely with users to ensure the success of experiments (experiment design, experiment conduct, data analysis, etc.) and receive input from them on potential new technical directions. This management configuration has worked successfully throughout the history of GSECARS.

Future APS Upgrade

The APS is planning an upgrade of the storage ring to a Multi-Bend Achromat (MBA) lattice. This upgrade will reduce the horizontal emittance of the machine by a factor of 40, which means a much smaller electron beam source size and divergence. This will greatly improve our ability to focus the x-ray beam into a small spot with high flux, and so will be a huge benefit to the microprobe and diamond anvil cell programs at GSECARS. This new $815M upgrade has made significant progress, and is on track in spite of the COVID-19 pandemic. The APS is scheduled to shut down for 12 months starting in June 2022, though there is some possibility this could slip by 6 months. The upgrade will provide a significant enhancement to the capabilities of the GSECARS facility. The storage ring energy will be reduced from 7 to 6 GeV, so the project will provide new optimized undulators to all the beamlines. To take maximum advantage of the improved source we will need to upgrade our focusing optics and detectors. We have included some funding for improved optics in the current 5-year cooperative agreement. We have also been informed that the APS Upgrade Project itself will fund a number of optics upgrades for GSECARS undulator beamlines, for a total of about $700K. This will allow us to use our NSF funding for the bending magnet optics, and for other components of the upgrade. Up-to-date information on the APS Upgrade project can be found at http://www.aps.anl.gov/APS-Upgrade/.

Science Highlights

We present here the abstracts of 10 papers published in Year 4 of this award using data collected at GSECARS. The complete list of all 170 publications from GSECARS for this year can be found at the end of this report.

The crystal structures of Fe-bearing $MgCO_3$ sp^2- and sp^3-carbonates at 98 GPa from single-crystal X-ray diffraction using synchrotron radiation

Publication: Stella Chariton, Maxim Bykov, Elena Bykova, Egor Koemets, Timofey Fedotenko, Björn Winkler, Michael Hanfland, Vitali B. Prakapenka, Eran Greenberg, Catherine McCammon, Leonid Dubrovinsky, ," **Acta Crystallogr. E** 76 (5), 715-719 (2020). DOI: 10.1107/S2056989020005411

The crystal structure of $MgCO_3$-II has long been discussed in the literature where DFT-based model calculations predict a pressure-induced transition of the carbon atom from the sp^2 to the sp^3 type of bonding. We have now determined the crystal structure of iron-bearing $MgCO_3$-II based on single-crystal X-ray diffraction measurements using synchrotron radiation. We laser-heated a synthetic $(Mg_{0.85}Fe_{0.15})CO_3$ single crystal at 2500 K and 98 GPa and observed the formation of a monoclinic phase with composition $(Mg_{2.53}Fe_{0.47})C_3O_9$ in the space group $C2/m$ that contains tetrahedrally coordinated carbon, where CO_4^{4-} tetrahedra are linked by corner-sharing oxygen atoms to form three-membered $C_3O_9^{6-}$ ring anions. The crystal structure of $(Mg_{0.85}Fe_{0.15})CO_3$ (magnesium iron carbonate) at 98 GPa and 300 K is reported here as well. In comparison with previous structure-prediction calculations and powder X-ray diffraction data, our structural data provide reliable information from experiments regarding atomic positions, bond lengths, and bond angles.

Phase transformation of hydrous ringwoodite to the lower-mantle phases and the formation of dense hydrous silica

Publication: Huawei Chen, Kurt Leinenweber, Vitali Prakapenka, Martin Kunz, Hans A. Bechtel, Zhenxian Liu, Sang-Heon Shim, **Am. Mineral.** 105 (9), 1342-1348 (2020). DOI: 10.2138/am-2020-7261

To understand the effects of H_2O on the mineral phases forming under the pressure-temperature conditions of the lower mantle, we have conducted laser-heated diamond-anvil cell experiments on hydrous ringwoodite (Mg_2SiO_4 with 1.1 wt% H_2O) at pressures between 29 and 59 GPa and temperatures between 1200 and 2400 K. Our results show that hydrous ringwoodite (hRw) converts to crystalline dense hydrous silica, stishovite (Stv) or $CaCl_2$-type SiO_2 (mStv), containing 1 wt% H_2O together with Brd and MgO at the pressure-temperature conditions expected for shallow lower-mantle depths between approximately 660 to 1600 km. Considering the lack of sign for melting in our experiments, our preferred interpretation of the observation is that Brd partially breaks down to dense hydrous silica and periclase (Pc), forming the phase assembly Brd + Pc + Stv. The results may provide an explanation for the enigmatic coexistence of Stv and Fp inclusions in lower-mantle diamonds.

Dynamic Biogeochemistry of the Particulate Sulfur Pool in a Buoyant Deep-Sea Hydrothermal Plume

Publication: Brandi R. Cron, Cody S. Sheik, Fotios-Christos A. Kafantaris, Gregory K. Druschel, Jeffrey S. Seewald, Christopher R. German, Gregory J. Dick, John A. Breier Jr., Brandy M. Toner, **Am. Mineral.** 105 (9), 1342-1348 (2020). DOI: 10.2138/am-2020-7261

In deep-ocean hydrothermal vent systems, oxidation–reduction (redox) reactions involving sulfur are known to fuel primary production via chemosynthesis. The particulate sulfur pool within buoyant hydrothermal plumes available to microorganisms as metabolic substrates remains undescribed. In this study, buoyant hydrothermal plume particles were collected from the Von Damm Vent Field, Mid-Cayman Rise, Caribbean. A novel in situ filtration system and remotely operated vehicle were used to collect samples along vertical profiles above two sites close to the summit of Mount Dent. Particulate sulfur speciation was measured using sulfur 1s X-ray absorption near edge structure (XANES) spectroscopy. The activity of sulfur-cycling genes in the buoyant plume was measured using metatranscriptomic sequencing. Our results indicate that both solid-state sulfur chemistry and microbial activity within the Von Damm buoyant plume are dynamic and diverse over short temporal and spatial scales. The particulate sulfur species and sulfur-cycling microbial communities generated in the buoyant plume are inputs to the neutrally buoyant plume and thus have potential for distant transport in the deep ocean. The buoyant plume particulate sulfur species include metal sulfides, thiol and organic monosulfide, thiophene, sulfone, sulfonate, ester sulfate, and sulfate. The microbial community carries a suite of active sulfur-cycling proteins (*dsr*AB, the sox enzyme complex, *sqr, psr, dpr*AB, and SAT). Should these materials be exported to the neutrally buoyant plume, they will have implications for deep-ocean biogeochemistry through sustained biomass production based on sulfur oxidation and reduction.

Elasticity of single-crystal Fe-enriched diopside at high-pressure conditions: Implications for the origin of upper mantle low-velocity zones

Publication: Dawei Fan, Suyu Fu, Chang Lu, Jingui Xu, Yanyao Zhang, Sergey N. Tkachev, Vitali B. Prakapenka, Jung-Fu Lin, **Am. Mineral.** 105 (9), 1342-1348 (2020). DOI: 10.2138/am-2020-7261

Diopside is one of the most important end-members of clinopyroxene, which is an abundant mineral in upper-mantle petrologic models. The amount of clinopyroxene in upper-mantle pyrolite can be ∼15 vol%, while pyroxenite can contain as high as ∼60 vol% clinopyroxene. Knowing the elastic properties of the upper-mantle diopside at high pressure-temperature conditions is essential for constraining the chemical composition and interpreting seismic observations of region. Here we have measured the single-crystal elasticity of Fe-enriched diopside ($Di_{80}Hd_{20}$, Di-diopside, and Hd-hedenbergite; also called Fe-enriched clinopyroxene) at high-pressure conditions up to 18.5 GPa by using in situ Brillouin light-scattering spectroscopy (BLS) and synchrotron X-ray diffraction in a diamond-anvil cell. Our experimental results were used in evaluating the effects of pressure and Fe substitution on the full single-crystal elastic moduli across the Di-Hd solid-solution series to better understand the seismic velocity profiles of the upper mantle. Using the third- or fourth-order Eulerian finite-strain equations of state to model the elasticity data, the derived aggregate adiabatic bulk and shear moduli (K_{S0}, G_0) at ambient conditions were determined to be 117(2) and 70(1) GPa, respectively. The first- and second-pressure derivatives of bulk and shear moduli at 300 K were $(\partial K_S/\partial P)_T = 5.0(2)$, $(\partial^2 K_S/\partial P^2)_T = -0.12(4)\ \mathrm{GPa}^{-1}$ and $(\partial G/\partial P)_T = 1.72(9)$, $(\partial^2 G/\partial P^2)_T = -0.05(2)\ \mathrm{GPa}^{-1}$, respectively. A comparison of our results with previous studies on end-member diopside and hedenbergite in the literatures shows systematic linear correlations between the Fe composition and single-crystal elastic moduli. An addition of 20 mol% Fe in diopside increases K_{S0} by ~1.7% (~2 GPa) and reduces G_0 by ~4.1% (~3 GPa), but has a negligible effect on the pressure derivatives of the bulk and shear moduli within experimental uncertainties. In addition, our modeling results show that substitution of 20 mol% Fe in diopside can reduce V_P and V_S by ~1.8% and ~3.5%, respectively, along both an expected normal mantle geotherm and a representative cold subducted slab geotherm. Furthermore, the modeling results show that the V_P and V_S profiles of Fe-enriched pyroxenite along the cold subducted slab geotherm are ~3.2% and ~2.5% lower than AK135 model at 400 km depth, respectively. Finally, we propose that the presence of Fe-enriched pyroxenite (including Fe-enriched clinopyroxene, Fe-enriched orthopyroxene, and Fe-enriched olivine), can be an effective mechanism to cause low-velocity anomalies in the upper mantle regions atop the 410 km discontinuity at cold subudcted slab conditions.

The seismically fastest chemical heterogeneity in the Earth's deep upper mantle—implications from the single-crystal thermoelastic properties of jadeite

Publication: Ming Hao, Jin S. Zhang, Caroline E. Pierotti, Wen-Yi Zhou, Dongzhou Zhang, Przemyslaw Dera, **Earth Planet. Sci. Lett. 543**, 116345 (2020). DOI: 10.1016/j.epsl.2020.116345

Jadeite is a major mineral phase (up to 50 vol%) in the subducted sediments/crust with continental origin, which are one of the major heterogeneities and important enriched geochemical reservoirs (such as EM-1 and EM-2) for incompatible elements in the Earth's interior. Identifying and locating the enriched geochemical heterogeneities requires knowledge of the elastic properties of relevant mineral phases at high pressure-temperature conditions. Unfortunately, the single-crystal elastic properties of jadeite have never been measured at high-pressure conditions, partially due to its low crystal symmetry. In this study, we have experimentally determined the single-crystal elastic moduli of jadeite at high pressures for the first time up to 18 GPa at the ambient temperature condition using Brillouin spectroscopy. Fitting the third-order finite strain equation of state to the velocity-pressure data yields KS0′=3.9(1), G0′=1.09(4) with ρ0=3.302(5) g/cm^3, K_{S0}=138(3) GPa, and G_0=84(2) GPa. In addition, we have also conducted synchrotron single-crystal X-ray diffraction experiments up to 25 GPa and 700 K. The fitting of a Holland-Powell type thermal-pressure Birch-Murnaghan equation of state yields KT0′=3.8(2) and α0=3.4(5) $\times 10^{-5}\ \mathrm{K}^{-1}$. Based on the obtained thermoelastic parameters of jadeite, the density and seismic velocities of continent-derived sediments/crust are modeled at the depth range from 200 to 500 km. The seismic velocities of the subducted continental sediments/crust become extremely fast at depths greater than ~300 km, up to 11.8% and 14.7% faster than the Vp and Vs of the ambient mantle, and 5.6% and 7.3% faster than the Vp and Vs of the subducted oceanic crust. The existence of even a small amount of the subducted continental sediments/crust can result in strong seismic anomalies in the Earth's interior.

A structural study of size-dependent lattice variation: In situ X-ray diffraction of the growth of goethite nanoparticles from 2-line ferrihydrite

Publication: Peter J. Heaney, Matthew J. Oxman, Si Athena Chen**, Am. Mineral. 105** (5), 652-663 (2020). DOI: 10.2138/am-2020-7217

Unlike most native metals, the unit cells of metal oxides tend to expand when crystallite sizes approach the nanoscale. Here we review different models that account for this behavior, and we present structural analyses for goethite (α-FeOOH) crystallites from ~10 to ~30 nm. The goethite was investigated during continuous particle growth via the hydrothermal transformation of 2-line ferrihydrite at pH 13.6 at 80, 90, and 100 °C using time-resolved, angle-dispersive synchrotron X-ray diffraction. Ferrihydrite gels were injected into polyimide capillaries with low background scattering, increasing the sensitivity for detecting diffraction from goethite nanocrystals that nucleated upon heating. Rietveld analysis enabled high-resolution extraction of crystallographic and kinetic data. Crystallite sizes for goethite increased with time at similar rates for all temperatures.

With increasing crystallite size, goethite unit-cell volumes decreased, primarily as a result of contraction along the *c*-axis, the direction of closest-packing (space group *Pnma*). We introduce the coefficient of nanoscale contraction (CNC) as an analog to the coefficient of thermal expansion (CTE) to compare the dependence of lattice strain on crystallite size for goethite and other metal oxides, and we argue that nanoscale-induced crystallographic expansion is quantitatively similar to that produced when goethite is heated. In addition, our first-order kinetic model based on the Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation yielded an activation energy for the transformation of ferrihydrite to goethite of 72.74 ± 0.2 kJ/mol, below reported values for hematite nucleation and growth.

Redox state of Earth's magma ocean and its Venus-like early atmosphere

Publication: Paolo A. Sossi, Antony D. Burnham, James Badro, Antonio Lanzirotti, Matt Newville, Hugh St.C. O'Neill**, Sci. Advances 6** (48), eabd1387 (2020). DOI: 10.1126/sciadv.abd1387

Exchange between a magma ocean and vapor produced Earth's earliest atmosphere. Its speciation depends on the oxygen fugacity (fO_2) set by the Fe^{3+}/Fe^{2+} ratio of the magma ocean at its surface. Here, we establish the relationship between fO_2 and Fe^{3+}/Fe^{2+} in quenched liquids of silicate Earth-like composition at 2173 K and 1 bar. Mantle-derived rocks have $Fe^{3+}/(Fe^{3+}+Fe^{2+})$ = 0.037 ± 0.005, at which the magma ocean defines an fO_2 0.5 log units above the iron-wüstite buffer. At this fO_2, the solubilities of H-C-N-O species in the magma ocean produce a CO-rich atmosphere. Cooling and condensation of H_2O would have led to a prebiotic terrestrial atmosphere composed of CO_2-N_2, in proportions and at pressures akin to those observed on Venus. Present-day differences between Earth's atmosphere and those of her planetary neighbors result from Earth's heliocentric location and mass, which allowed geologically long-lived oceans, in-turn facilitating CO_2 drawdown and, eventually, the development of life.

High-pressure elastic properties of dolomite melt supporting carbonate-induced melting in deep upper mantle

Publication: Man Xu, Zhicheng Jing, Suraj K. Bajgain, Mainak Mookherjee, James A.Van Orman, Tony Yu, Yanbin Wang**, Proc. Natl. Acad. Sci. USA 117** (31), 18285-18291 (2020). DOI: 10.1073/pnas.2004347117

Petrologic studies suggest that carbonate-rich melts are present in the Earth's upper mantle and play an important role in the deep carbon cycle. However, seismic detection of these melts is difficult due to the lack of understanding of the elastic properties of carbonate melts. Here we determined the sound velocity and density of dolomite melt at upper mantle conditions using high-pressure experiments and theoretical simulations. The calculated velocities of carbonate melt-bearing mantle using these new elasticity data were compared with global seismic observations. The result suggests that ~0.05% carbonate-rich melt can be pervasively present in the deep upper mantle, implying a global average mantle carbon concentration of 80-140 ppm.

Low Melting Temperature of Anhydrous Mantle Materials at the Core-Mantle Boundary
Publication: Taehyun Kim, Byeongkwan Ko, Eran Greenberg, Vitali Prakapenka, Sang-Heon Shim, Yongjae Lee**, Geophys. Res. Lett. 47** (20), e2020GL089345 (2020). DOI: 10.1029/2020GL089345

One of the central challenges in accurately estimating the mantle melting temperature is the sensitivity of the probe for detecting a small amount of melt at the solidus. To address this, we used a multichannel collimator to enhance the diffuse X-ray scattering from a small amount of melt and probed an eutectic pyrolitic composition to increase the amount of melt at the solidus. Our in situ detection of diffuse scattering from the pyrolitic melt determined an anhydrous melting temperature of 3,302 ± 100 K at 119 ± 6 GPa and 3,430 ± 130 K at the core-mantle boundary (CMB) conditions, as the upper bound temperature. Our CMB temperature is approximately 700 K lower than the previous estimates, implying much faster secular cooling and higher concentrations of S, C, O, and/or H in the region, and nonlinear, advocating the basal magma ocean hypothesis.

Exploring the effect of flow condition on the constitutive relationships for two-phase flow
Publication: Douglas E. Meisenheimer, James E. McClure, Mark L. Rivers, Dorthe Wildenschild**, Adv. Water Resour. 137**, 103506-1-103506-10 (2020). DOI: 10.1016/j.advwatres.2020.103506

Empirical relationships that describe two-phase flow in porous media have been largely hysteretic in nature, thereby requiring different relationships depending on whether the system is undergoing drainage or imbibition. Recent studies have suggested using interfacial area to close the well-known capillary pressure-saturation relationship, while others expand upon this by including the Euler characteristic for a geometric description of the system. With the advancement of fast x-ray microtomography at synchrotron facilities, three-dimensional experiments of two-phase quasi- and non-equilibrium flow experiments were conducted to quantify the uniqueness of constitutive relationships under different flow conditions. We find that the state functions that include the Euler characteristic provide the most unique prediction of the state of the system for both quasi- and non-equilibrium flow. Of these functions, those that infer volume fraction from the other state variables are independent of flow condition (quasi- or non-equilibrium). This enhances the applicability of new constitutive relationships allowing for more robust models of two-phase flow.

GSECARS Publications 2020
Total 159 journal articles, 10 Ph.D theses, and 1 masters thesis

Journal Articles

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Ph.D Theses

1. Jiadi Fan, "Atomistically-Informed Finite Element Simulations of Phase Transformations and Fracture in Materials," Ph.D., University of Minnesota, 2020.
2. Curtis L. Johnson, "The Relationship Between Eocene Magmatism and Gold Mineralization in the Great Basin, USA: Insights from the Phoenix-Fortitude Porphyry-Skarn System and Regional Intrusions Associated with Mineralization," Ph.D., University of Nevada, Reno , 2020.
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Masters Theses

1. Jason Ott, "METASTABILITY OF TREMOLITE AT HIGH PRESSURES AND TEMPERATURES," Masters, UNIVERSITY OF CALIFORNIA SANTA CRUZ, 2020.