Russell J. Hemley
The George Washington University
School of Engineering and Applied Science
Washington, DC 20052

SSAP Symposium, Albuquerque, NM - February 19-20, 2019
I. Overview
   MOTIVATION, CENTER STRUCTURE, PERSONNEL

II. Training
   EDUCATION, OUTREACH RESEARCH TRAINING

III. Selected Science
   STUDENT AND NNSA LAB PROJECTS
Materials at High Pressure

I. OVERVIEW

Exploring Energy Landscapes

>100’s GPa (to ~TPa)

~ eV energies
valence electrons

~ keV energies
core electrons

>100’s Mbars (1 Gbar)
Energetic photon/particle flux
Chemical extremes
Electromagnetic extremes
Pressures and temperatures
I. OVERVIEW

1. Phase Stability

2. Aging

3. Corrosion Reactions
Mission of CDAC: 2018-2023

- To enhance our understanding of a broad range of materials in extreme pressure-temperature ($P-T$) regimes;

- To integrate and coordinate static compression, dynamic compression, and theoretical studies of materials;

- To train the next generation of scientists for work in this field by enriching graduate education and training and by facilitating interactions between NNSA laboratory scientists and academia.
• How can we understand, predict, and control the behavior of matter and materials to very high compressions?
• What new physics may emerge in ‘cold’ to ‘warm’ dense matter?
• How can we accurately determine fundamental thermodynamic and kinetic properties up to high $P-T$ multimegabar conditions?
• How do defects, grain boundaries, and interfaces respond to high $P-T$ conditions and as a function of strain rate?
• How can we better measure time-dependent transformations, and bridge strain-rate gaps in static and dynamic compression?
• Can we better determine constituitive properties such as strength, plasticity, and rheology at ultrahigh $P-T$ conditions?
• Can we expand the materials synthesis frontier to very high $P-T$ conditions to produce new, optimized materials?
Mission of CDAC – 2018-2023

I. OVERVIEW
Components of the Center

Academic Partners

- GEORGE WASHINGTON (Hemley)
- CALTECH (Fultz)
- MICHIGAN STATE (Dorffmann)
- NORTHWESTERN (Jacobsen)
- UNIV. at BUFFALO (Zurek)
- UNIV. CALIF. – BERKELEY (Jeanloz)
- UNIV. ILLINOIS (Dlott & Ertiken)
- UNIV. TENNESSEE (Lang)
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CDAC Personnel

• Manage facilities
• Student/postdoc mentoring
• Visitor training
• Technique development

Core Personnel

Steve Gramsch
Deputy Director/Outreach Coordinator

Maddury Somayazulu
Chief Scientist/Senior Lab Manager

Muhtar Ahart
Research Scientist Experiments

Zhenxian Liu
Beamline Scientist NSLS II (NSF-support)
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Academic Collaborators
OTHER UNIVERSITY GROUPS
FACILITY USERS

NNSA Laboratory Partners
ALL HIGH P-T GROUPS AT LLNL, LANL, SNL;
STEERING/ADVISORY COMMITTEE MEMBERS

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CDAC facilitates high $P-T$ experiments at HPCAT and at other facilities at APS
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**Evolution of HPCAT and CDAC**

1988 High-Pressure Opportunities
   ANL Report

1995 Feasibility studies at X17C (NSLS), GSECARS (APS)

1998 ‘HPCAT Concept’ proposed

1999 HPCAT launched with CIW, UNLV, and LLNL

2003 CDAC launched

2006 Expanded capabilities (dynamic)

2009 EFree support lab at APS

2013 Trilab (LLNL, LANL, SNL)

2018 LLNL/NNSA/APS management

2022 APS and HPCAT upgrades
CDAC facilitates high $P-T$ experiments at HPCAT and at other facilities at APS

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2022 APS and HPCAT upgrades
CDAC manages and coordinates activities at major facilities for high $P$-$T$ research

- Major component of CDAC
- Academic and NNSA Lab users (e.g., LANL, SNL, LLNL)

- Frontier Infrared Spectroscopy (FIS) beamline: first synchrotron IR facility at NSLS-II with over 1000 ft$^2$ space
- Beamline under commissioning, general user beam available in May, 2019
- 50% available GU beamtime including 10% PU beamtime for CDAC, new opportunities for NNSA labs and SSAAP.
CDAC supports and promotes research activities at other major DOE facilities
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I. OVERVIEW

LANSCE

Z

NIF

OMEGA

CDAC

APS

HPCAT, DCS
GSECARS...

SNS

SNAP,
VISION...

NSLS-II

FIS, MET,...

LCLS

MEC,...
- Supported 18 PhD students – 10 PhDs awarded
- 68 total PhDs awarded with CDAC support
- 8 early career scientists join DOE/NNSA labs
  - Bethany Chidester (Chicago) to SNL
  - Eloisa Zepeda-Alarcon (Berkeley) to LANL
  - John Lazarz (Northwestern) to LANL
  - Andrew Shamp (Buffalo) to NNSA HQ to LLNL
  - Samantha Clarke (Northwestern) to LLNL
  - Will Bassett (Illinois) to LLNL
  - Sakun Dawal (WSU) to SNL
  - Ken O’Neil (Tennessee/FIS) to LANL

- Student and Faculty Awards
  - Sakun Duwal (NASA; WSU Golding Scholarship; WSU Seminar Award)
  - Will Bassett (AIRAPTJamieson Award)
  - Erin Nissen (NNSA Fellowship)
  - Lowell Miyagi (NSF CAREER grant)
  - Brent Fultz (APS Fellowship)
  - Russell Hemley (Marker Lecturer, PSU; Sack Lecturer, Cornell; S&T Lecturer, SNL)

- 31 Students/Postdocs to positions in DOE/NNSA Labs since 2003
Educational Enrichment at NNSA Laboratories

CDAC Student Samantha Couper will work at LLNL to learn ALE3D multi-physics simulations in order to simulate low symmetry high strain deformation and study stress strain heterogeneity in aggregates with a symmetry and strength contrast.

CDAC student Hannah Bausch is developing a project at SNL with staff scientists (and former CDAC students) Chris Seagle and Joshua Townsend to study ramp-wave compression of (Mg,Fe)O on THOR.

CDAC student affiliate Erin Nissen worked with staff scientist Dan Dolan this summer at SNL on THOR to study the quasi-isentropic compression of liquid water.

CDAC student Jane Herriman has been investigating $P$-$T$ effects in GaN to understand structure-property relations and anharmonicity at LLNL.
Hannah Bausch (Northwestern) – Shock Properties and Equations of State of (Mg,Fe)O up to TPa Pressures
Camille Bernal (Caltech) – Non-Harmonic Interactions in bcc Chromium
Tiang Bi (Buffalo) – Crystal Structure and Properties of Hydrogen Rich Materials at High Pressure
Brian Blankanau (Illinois) – NiTi and CuZnAl Shape Memory Alloys Under Extreme Loading Conditions
Ben Brugman (Michigan State) – Natural Variability in the Dynamic Strength of Chondrites and Implications for Asteroid Hazard Mitigation
Samantha Couper (Utah) – Texture and Anisotropy of Brigemanite and Ferropericlase at Lower Mantle Conditions
Will Cureton (Tennessee) – Probing the Defect Structure in UO₂ Induced by Dense Electronic Excitation
Jane Herriman (Caltech) – Phonon Thermodynamics and Elastic Behavior of GaN and GaAs at High Temperatures and Pressures
Larry Salvati (Illinois) – Probing Shock Initiation of Plastic Explosives With a Tabletop Microscope

Two Posters by Former CDAC Students

Jeff Pigott (LANL) – Development of Advanced High Pressure Experimental Capabilities for Studying Materials at Extreme Conditions and Supporting the LANL-NNSA Mission
Jinhyuk Lim (WSU) – Equation of State of Dense H₂-He Mixtures to 160 GPa: Comparison With Pure H₂ and He
Selected Topics

1. Metals and Metal Alloys
1. Dynamic Compression
1. Defects and Deformation
1. New Materials
1. Novel Phenomena

2017-2019: 167 Publications (including in press)
- 23 Student papers (12 Student First Author Papers)

Since 2003: 1920+ Publications
(280+ Student Publications)
Experimental and computational studies of phonons and magnons in metals
Magnon-Phonon Interactions in Pd$_3$Fe

- Measured and calculated phonons across magnetic transition under $T$.

Phonons calculated with $T$-dependent potentials using VASP. Magnetism included in spin-polarized DFT.

Anharmonicity and magnon-phonon interactions compete with each other, partly cancelling.

[Yang et al., Phys. Rev. B (2018)]
Magnon-Phonon Interactions in Pd₃Fe

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[Yang et al., Phys. Rev. B (2018)]

(a) NRIXS $^{57}$Fe phonon DOS at 298 and 786 K.
(b) Calculated curves at 300 and 800 K. NRIXS and XRD measured at HPCAT.

Non-Harmonic Phonons in Cr

- Major discrepancies in magnitude and sign of quasiharmonic phonons.
- Very large non-harmonic contributions that vary with phonon polarizations.

Phonon DOS curves of Cr from inelastic neutron scattering measurements at ARCS at the SNS.
Modeling mechanical response of shape memory alloys under high pressure and high strain rates
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Shape Memory Effects

Elif Ertekin
(Illinois)
Modeling mechanical response of shape memory alloys under high pressure and high strain rates

Shape Memory Effects

Example: Ni$_2$FeGa

Prior work:
- mechanical response of heusler shape memory materials
- optimizing magnetocaloric effect

Program goals:
- shape memory effect under pressure
- strain-rate dependence of stress-strain response
- Influence of microstructure on transmission of transformation fron
Table-top dynamic compression: New microscope with high temporal and spatial resolution
Table-top dynamic compression: New microscope with high temporal and spatial resolution

Flyer plates 0-6 km/s. Measures pressure, density, temperature, composition, microstructure
Table-top dynamic compression: New microscope with high temporal and spatial resolution

Recent accomplishments

- Detonation on a tabletop
- Real-time imaging of hot spots in plastic explosives
- Cellular structure in detonating nitromethane for rapid measurements of reaction zone
- Direct absorption of electron plasma in detonation front
- Temperature measurements of shocked TATB
- ALE3D simulations of flyer launch and impact

Flyer plates 0-6 km/s. Measures pressure, density, temperature, composition, microstructure

Dana Dlott
Larry Salvati
Erin Nissen

Illinois - LLNL
**Mid-scale shock compression: Dynamic strength of heterogeneous materials - chondrites**

**TRIDENT, JANUS, JUPITER**

- Strength to be used in asteroid hazard mitigation models
- Microanalysis of recovered samples conducted in support of interferometry analyses
- Proposed work at JLF in 2019:
  - reduce effects of grain heterogeneity
  - systematic evaluation of the effects of composition

Experimental setup at JLF (Janus), LLNL: use structure of low-energy laser shock to constrain dynamic strength

**Shock produces cracks, ablation features**

- Heterogeneity in grain size and orientation complicates analysis

**Michigan State University**

Ben Brugman

Susana Dorfman

Michigan State - LLNL
Large-scale shock compression: Discovery Science Campaigns
1. Hydrogen ‘PPT’ Fluid Transition

2. Hydrogen near melting to TPa pressures

2. Fe Melting to 2 TPa in ‘habitable’ exoplanets
Insulator-metal transition in fluid deuterium at NIF

Dynamic Compression

III. SCIENCE

REFLECTIVITY

4 SHOTS

ABSORPTION

CONDUCTIVITY

Temperature (K)

Pressure (GPa)

Crystalline solid phases

Metallic fluid

H₂ → H

Molecular fluid

Static

Z Pinch

Theory

[Celliers et al., Science (2018)]

Actinide Materials under Extreme Conditions

III. SCIENCE

Defects and Deformation
Actinide Materials under Extreme Conditions

III. SCIENCE
Defects and Deformation

Large Ion Accelerator Facility
Simulation of radiation effects in actinide materials

Spallation Neutron Source
Structural characterization via neutron total scattering

maximization of irradiated sample volume
very high energy ions (GeV energies)

minimization of required sample volume
very intense neutron beam ($10^8$ neutrons/cm$^2$/sec)
**Actinide Materials under Extreme Conditions**

**Technique Development:** Combining world’s largest ion accelerator facility with world’s most intense spallation neutron source led to first neutron characterization of ion-irradiated materials.

![Large Ion Accelerator Facility](image1)

- Simulation of radiation effects in actinide materials

![Spallation Neutron Source](image2)

- Structural characterization via neutron total scattering

- Maximization of irradiated sample volume
- Very high energy ions (GeV energies)
- Minimization of required sample volume
- Very intense neutron beam ($10^8$ neutrons/cm²/sec)

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**III. SCIENCE**

**Defects and Deformation**

- **Novel insight into local structure of irradiated materials**

*References*

- Palomares, et al. *Inorganic Chemistry*, in review
Radiation damage under pressure: Thermally induced coloration of compressed KBr
Radiation damage under pressure: Thermally induced coloration of compressed KBr

Optical images of defect-damaged KBr during decompression. Images were taken while at pressure in a LHDAC using both reflected and transmitted light. At 58 GPa (a) before heating, and (b) after heating. (c)–(f) Upon decompression, the defect-damaged KBr becomes less absorbing, progressing from black to orange, to blue after the B2 to B1 phase transition at $\sim 1.8$ GPa, and eventually returning to transparent at room pressure.

High-pressure visible absorbance spectra for defect-damaged KBr samples after quenching from high temperature.

Measurements carried out at the IR Lab, NSLS-II

[Arveson et al., Phys Rev B (2018)]
High $P$-$T$ Deformation of Aggregate Materials

Deformation to 36 GPa at 1000 K

$\text{MgSiO}_3$  (Mg,Fe)$\text{O}$

$$\text{Elasto-Visco Plastic Self Consistent Method}$$

$(100)[010] + (100)<011>$

Samantha Couper

[Couper et al, to be submitted]

Utah - ALS
HIGH P-T DEFORMATION OF AGGREGATE MATERIALS

Deformation to 36 GPa at 1000 K

MgSiO₃  (Mg,Fe)O

Elasto-Visco Plastic Self Consistent Method

(100)[010] + (100)<011>

Utah - ALS

[Couper et al, to be submitted]
Discovery of New Intermetallic Phases Under Pressure
Discovery of New Intermetallic Phases Under Pressure

Northwestern-HPCAT

FeBi$_2$  MnBi$_2$

Discovery of Cu$_3$Pb

[ACS Central Science (2016); submitted]

James Walsh


Alexandra Tamerius

Controlling Dimensionality in the Ni–Bi System with Pressure

[Chem. Materials (2019)]

Samantha Clarke
Now at LLNL
Additive manufacturing and inkjet printing of energy materials
Additive manufacturing and inkjet printing of energy materials

Additive Laser Manufacturing of Thermoelectric Bi$_2$Te$_3$

- First-ever successful additive processing on loose powders of thermoelectric materials to make bulk parts with adaptable geometry
- Achieved: 88% relative density; preserved crystal structure; reasonable thermoelectric and electrical properties


All-carbon Flexible Electronics: Inkjet Printing of Multilayer Graphene Nanospheres

- Carbon negative material synthesis
- Electrostatically stabilized ink
- Achieved electrical percolation

[M. Orrill et al. (in preparation)]
Diamond clad fiber fabrication by microwave plasma CVD

- Optical fibers sensors for monitoring chemical & biological parameters in harsh environmental conditions.
- Uniform coating and high quality diamond are indicated by SEM and Raman measurements.
- Size of fiber diameters ranges from 50 to 300 µm with diamond facet crystal growth encapsulation.

High-pressure spectroscopy of multiferroic Ni$_3$TeO$_6$
High-pressure spectroscopy of multiferroic Ni$_3$TeO$_6$

300 K crystal structure of Ni$_3$TeO$_6$ and schematic view of the spin pattern and super-exchange interactions in Ni$_3$TeO$_6$.

A decrease in compressibility near 4 GPa that can be traced to a rather surprising tendency in a specific local lattice distortion.

Ken O’Neal
Univ. Tenn. Grad. Student
NSLS IR User, now at LANL Postdoc

Experimental and theoretical studies of new hydride materials
Experimental and theoretical studies of new hydride materials

- CaH$_{2.5}$ and CaH$_4$, containing H$_2$ units with stretched bonds and H$^-$

- H$_2$ $\sigma \rightarrow$ metal $d$, and metal $d \rightarrow$ H$_2$ $\sigma^*$ back-bonding elongates the H-H bonds


GWU-Buffalo-HPCAT
CaH$_{2.5}$ and CaH$_4$, containing H$_2$ units with stretched bonds and H$^-$

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GWU-Buffalo-HPCAT

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GWU-Buffalo-HPCAT

Periodic Table of Superconducting Hydrides

Predicted high $T_c$ superconductivity in compressed lanthanum and yttrium hydrides

Can we accurately predict and experimentally confirm room temperature superconductivity?

$L_c$ as a function of pressure

$\mu^*=0.1$  $\mu^*=0.13$

LaH$_{10}$  YH$_{10}$

Can we accurately predict and experimentally confirm room temperature superconductivity?

Laser heated La + H$_2$

X-RAY DIFFRACTION

Carnegie-GWU-HPCAT

Hanyu Liu  Ivan Naumov  Roald Hoffman  N.W. Ashcroft

[II. SCIENCE  Novel Phenomena]

Hanyu Liu  Ivan Naumov  Roald Hoffman  N.W. Ashcroft

Carnegie-Cornell-GWU

[Zachary Geballe]

[Liu et al., PNAS (2017)]

[Roald Hoffman N.W. Ashcroft]

[Carnegie-Cornell-GWU]

[Geballe et al., Angew. Chem. (2018)]
Superconductivity above 260 K LaH$_{10}$

Superconductivity above 260 K LaH$_{10}$

Superconductivity above 260 K LaH$_{10}$

Critical current $J_c > 10^4$ A/cm$^2$

Complete ‘in situ’ measurements carried out at HPCAT

New era of research and discovery in superconductivity

Novel Phenomena

LaH$_{10}$ at 195 GPa

A direct result of NNSA investment in fundamental science

267 K in Albuquerque now

- room temperature superconductivity
CONCLUSIONS

1. **Education and Training**
   - Diverse student program with a large group of university partners
   - Continued placement of personnel in NNSA labs

2. **Science Program**
   - Continued growth in number of high-profile publications
   - New opportunities for materials dynamics under extremes
   - Novel phenomena uncovered at extreme conditions

3. **Prospects for Enhanced Partnerships**
   - Continued developments to support NNSA labs
   - New x-ray techniques (imaging, time-resolved, static/dynamic)
   - Opportunities for coordination across DOE facilities
BACKUP SLIDES
Integration of Experiment and Theory

Students from all three departments collaborate during recent HPCAT beamtime

3. SCIENCE

Steve Jacobsen (Geophysics)
Danna Freedman (Chemistry)
Chris Wolverton (MatSci)

Machine learning directed search for superhard materials

![Graph](image)

[Tehrani et al. JACS (2018)]

[Argonne National Laboratory]

[Exploring the High-Pressure Materials Genome](https://doi.org/10.1103/PhysRevX.8.041021)

**Maximilian Amsler,**¹,² Vinay I. Hegde,¹³ Steven D. Jacobsen,¹² and Chris Wolverton¹

¹Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, USA
²Department of Earth and Planetary Sciences, Northwestern University, Evanston, Illinois 60208, USA
Actinide Materials under Extreme Conditions

**Chemical Composition**

Neutron total scattering (SNS) and RMC modeling → simple defect structure in UO$_2$+x

R.I. Palomares et al. Inorganic Chemistry (under review)

**Dense Electronic Excitations**

Defect formation in actinide oxides depends on cation redox behavior and grain size


**High Temperature**

Local distortions in defective ThO$_2$ (diffuse scattering) recover at high temperature

Strength, elasticity and texture of soft and hard materials

**Strength of rare gas solids: effects of atomic number and fcc-hcp phase transition**

- Plot Data: He, Ne, Ar Ruby Data: Klotz et al., 2009, He: Singh et al., 2012, Ne: Dorfman et al., 2012, Ar: Mao et al., 2006

**Tungsten carbide at 66 GPa: diffraction pattern and full-profile refinement**

- Ruby Pressure Standard Deviation (GPa) vs. Average Pressure (GPa)
- Differential Stress (GPa) vs. Average Pressure (GPa)

**Symbols:**
- Xe
- Ar
- Ne
- Kr

**Note:** Kr similar to Ne and He

**Author:** Ben Brugman (Michigan State)


**Future plans**

High speed photography of hot spot growth and decay in shocked plastic explosives

Metallization at the shock front

Chemistry of extreme states of water

Shock-to-detonation in TATB initiated with PETN booster

Development of higher-speed flyer plate launcher

Hot spots in shocked single crystals

Movie of hot spots in 0.5 mm shocked HMX crystal
Rus, thought you might like these images.
Credit: Max Amsler (Cornell)
Collaborations with Experimental Groups

- Confirmed the experimental SiO₂ X-I model that does not invoke vacancy defects or partial occupancies.


- Molecular dynamics simulations of the photovoltaic methylammonium-lead-bromide (MAPbBr₃) revealed that the dynamics of the organic molecules and the inorganic lattice, coupled via the N-H···Br hydrogen-bonding interactions, affects the Pb-Br distance and the band gap evolution under pressure.

Table II. CDAC Academic Partners to Date

- Prof. David Cahill (Illinois) – 2010-2015
- Prof. Dhanesh Chandra (Nevada-Reno) – 2006
- Prof. Przemek Dera (Hawai‘i-Manoa) – 2013-2017
- Prof. Dana Dlott (Illinois) – 2003-2017
- Prof. Susannah Dorfman (Michigan State) – 2016-2017
- Prof. Robert Downs (Arizona) – 2008-2010
- Prof. Tom Duffy (Princeton) – 2003-2012
- Prof. Rodney Ewing (Michigan/Stanford) – 2010-2012
- Prof. Brent Fultz (Caltech) – 2003-2017
- Prof. Dion Heinz (Chicago) – 2003-2009, 2016-2017
- Prof. Toshiko Ichye (Georgetown) – 2015-2016
- Prof. Steven Jacobsen (Northwestern) – 2008-2017
- Prof. Abby Kavner (UCLA) – 2008-2015
- Prof. Maik Lang (Tennessee) 2016-2017
- Prof. Kanani Lee (New Mexico State/Yale) – 2006-2015
- Prof. Jie Li (Michigan) – 2008-2012
- Prof. Jung-Fu Lin (Texas-Austin) – 2009-2012
- Prof. Yanzhang Ma (Texas Tech) – 2006-2007
- Prof. Wendy Mao (Stanford) – 2008-2012
- Prof. Lowell Miyagi (Utah) – 2013-2017
- Prof. Wendy Panero (Ohio State) – 2008-2012
- Prof. Surendra Saxena (Florida International) – 2006-2012
- Prof. James Schilling (Washington at St. Louis) – 2008-2017
- Prof. Yogesh Vohra (Alabama-Birmingham) – 2003-2017
- Prof. Hans-Rudolf Wenk (Berkeley) – 2003-2017
- Prof. Jeff Yarger (Arizona State) – 2006-2012
- Prof. Choong-Shik Yoo (Washington State) – 2013-2017
- Prof. Eva Zurek (SUNY Buffalo) – 2013-2017
Actinide Materials under Extreme Conditions

Awards
R. Palomares: UTK Chancellor’s 2018 Extraordinary Professional Promise Award
R. Palomares: UTK, NE 2018 PhD Graduate Student Award
M. Lang: UTK, 2017 Tickle College of Eng. Professional Promise in Research Award
M. Lang: UTK, Tickle College of Eng., Pietro F. Pasqua Fellow Award, 2017

Publications
1. R.I. Palomares et al.: Oxygen point defect accumulation in single phase $\text{UO}_2+x$, Inorganic Chemistry (under review)
5. J.M. Heuser, et al.: Structural characterization of (Sm,Tb)PO$_4$ solid solutions and pressure induced phase transitions, J. European Ceramic Society 38, 4070-4081 (2018)
Need for Next Generation Materials

- Design, discovery, synthesis, and deployment of new materials
- Enhancing performance and lifetime of known materials
Coordinated Program of Extreme Conditions Science at the APS

First Proposed in 2013

The HPSynC Model
- Small, flexible research team with varied expertise
- Collection of portable instruments for working at various sectors
- Highly collaborative structure
- Basic infrastructure for high P-T research
- Development mode—pushing the frontier

APS Upgrade Priorities NNSA
- Real Materials: Defects, Alloys, Composites, Nanomaterials
- Real Conditions: High P-T, Strain, Strain Rate
- Real Time: Mechanistic studies of physical/chemical processes
- A fully upgraded HPCAT is an essential cornerstone of the effort

HPCAT
DCS
Other CATs
XSD

Other facilities (LCLS, NSLS-II, NIF, Z, Omega, MaRIE, …)

Question 4
Future Research Agenda

1. Coupling of multiple extreme conditions

Irradiating materials in diamond-anvil cells
⇒ Explore novel material phases that form under combined pressure and dense electronic excitations

Using HDAC as unique sample chamber for in situ synchrotron X-ray characterization (XRD and XAS)
⇒ Corrosion studies of nuclear materials as a function of temperature, stress, and aqueous solution

2. Investigating actinide-dense materials under extremes

uranium carbides
uranium nitrides

⇒ behavior of dense uranium materials under irradiation, temperature, etc…

http://enacademic.com/dic.nsf/enwiki/1749145
High $P$-$T$ Transitions in Hydrogen

CHANGE IN MELTING LINE BY HIGH P-T RAMAN

- Insulating to conducting fluid?
- Clarify discrepancies?
- Dissociation: $H_2$ to $H$?
- Jovian magnetic field generation?


National Ignition Facility, Lawrence Livermore National Laboratory

LASER DRIVEN DYNAMIC (RAMP) COMPRESSION

168 of 192 Beams Used
1.6 MJ Total Energy
WHY PRESSURE?

• 60 orders of magnitude in the universe
• Laboratory pressures
  - >100’s GPa (static), > 100 Mbar (dynamic)
• Varying atomic distances
  - Large compressions $\rho/\rho_0 > 10$
• Tuning properties
  - free energies and energy landscapes
• Numerous transformations
  - structural/electronic/magnetic
• Discovery of new phenomena
• New materials
  - recovery for applications

➤ Multiple extreme environments: $P$, $T$, $X$, $H$,…
Pressure effects on energy landscapes of complex polymers

- $P$-$T$ fluctuations function of $\kappa_T$ & $\alpha_P$

- Above $T_g$:

$$d^2(P, T) = d_0^2 \frac{T}{T_0} \left[ \exp(-\alpha_{P,0} T)(1 + \mu \kappa_{T,0} \Delta P)^\gamma \right]$$

$\gamma$ is Grüneisen and $m$ & $n$ are Mie potential parameter

- Below $T_g$:

$$d^2(P, T) = d_0^2 \frac{T}{T_0} \left[ \exp(-\alpha_{P,0}(T_g(P) - T_0))(1 + \mu \kappa_{T,0} \Delta P)^\gamma \right]$$

$$T_g(P) = T_{g,0} - \frac{1}{c\alpha_{P,0}} \log(1 + c\kappa_{T,0} \Delta P)$$

Pressure affects energy landscape by narrowing energy wells and by lowering barriers between substates

Lysozyme

Georgetown-Carnegie-GWU

Toshiko Ichiye
New tools have opened a new world on materials behavior under extreme $P-T$ conditions.