Chemistry in Planetary Materials under Extreme Pressure-Temperature Conditions


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**Goals**: Novel states and chemistry of planetary materials under extreme conditions

- **Scientific**: Investigate novel states and chemistry of dense planetary materials under extreme conditions, and develop enabling new high PT technologies

- **Education, Training and Workforce Development**:
  - Provide hand-on trainings for 6 GS, 2 US, and 2 PD
  - Sakun Duwal (PhD, 2018) Sandia National Laboratory
  - YoungJay Ryu (PhD, 2016) Univ. of Chicago-GESCARS
  - Ranga Diaz (PhD, 2014) Univ. of Rochester

- **Collaboration with National Laboratories**:
  - LLNL (W. Evans, Z. Jenei): dynamic-DAC at XFEL
  - LANL (D. Dattelbaum): Shocked carbon at LCLS
  - SNL (S. Duwal, C. Seagal): HEDM

- **Publication**: Five in 2019-2020
Approach: Study extreme materials behavior using enabling HP technologies and advanced 3G and 4G light sources.

3G Synchrotron X-ray

High Power Laser

Gas Guns

Dynamic-DAC

4G X-ray Free Electron Laser

Strain rate
Progress: Phase diagram, structure and transition in dense H₂-He mixtures

Binary phase diagram

Lim & Yoo, PRL (2018)

Structure and EOS

Lim & Yoo, PRB (2020)

Nucleation and Growth

Howard & Yoo, in progress

He EOS becomes softer in H₂-He mixtures likely due to lattice distortion in the hcp basal plane
Chemistry in He/H₂ mixtures with N₂/H₂O/Ne

1% N₂ in He

Small He cluster capturing N₂ upon He solidification

He/H₂-H₂O

Symmetric Ice X formed in H₂-H₂O mixture

He-Ne

Novel inert-gas alloy HeNe₂ formed in He-Ne
Recovered COH solid is highly stable at ambient condition, predominantly made of C-O single bonds (~3.2 g/cm³)

Material transformations under dynamic loadings

Dynamic-DAC complements conventional DAC and shock wave experiments,

Dynamic-DAC

Trapezoidal Saw
Sine wave etc.

PA Input

\[ \frac{\Delta P}{\Delta t} \]

\[ \sigma \]

\[ \dot{\varepsilon}_{cr} \]

\[ \sigma_{y} \]

\[ \sigma_{y} \]

\[ \sigma_{y} \]

\[ \Delta P \]

\[ f \]

\[ P_{\text{static}} \]

\[ V \]

\[ \Delta \]

\[ \text{time} \]
Chemistry at dense solid/liquid-solid interfaces: kinetically stabilized metastable ice phases

We use **dynamic-DAC** to investigate solid interface, metastable phase, and kinetic controlled process under precisely controlled pressures and compression rates.

**Refs:** Lee et al. PRB (2007), PNAS (2007); Evans et al. RSI (2008); Chen et al., PNAS (2011); Kim et al., PNAS (2019)
Probing structural evolution and metastable phases of $\text{H}_2\text{O}$ in dynamic-DAC using time-resolved x-ray diffraction

Experiments are in progress at HPCAT/APS and P2.2/PETRA-III
Catching atoms in transition using XFEL

- Isochoric heating by XFEL x-ray pulse (25 fs)
- Laser shock compression by high energy laser (100 J, 10 ns)
- Dynamic compression using dynamic-DAC, across phase changes
New “core-electron” chemistry at TPa

Exotic Conducting States predicted:
- Metallic H2
- Metallic diamond
- Metallic salt
- Metallic He
- Electrides
- Superionic water
- Etc. etc

High-PT research windows novel state, structures, bonding, and new chemistry that may occur in deep interiors of the Earth and Giant planets

Yoo, MRE (2020)
Exploit novel metallic phases of NaCl with predominantly ionic structures at NIF-accessible pressure.

Chen & Ma, EPL 100, 26005 (2012).

Four NIF-DS shots on ramp-compressed NaCl have been scheduled in FY2021-22;
C.S. Yoo, M. Kim, A. Howard - WSU;
C. Picard- Cambridge; E. Reed- Stanford;
M. Marshall, A. Jenei, J. Eggert, D. Swift - LLNL
Summary of progresses

Scientific Progresses:

• Determined phase diagram and EOS of He-H$_2$ mixtures

• Chemistry of quantum solids (H$_2$ and He) with other elemental solids including He, H$_2$, H$_2$O, N$_2$, C(graphite), CO, CO$_2$

• Synthesis of HED extended solid stable at ambient conditions: transparent high-density COH$_x$ network glass- the first 3D hydrocarbon polymer

• Dynamic crystallization and shock crystal growth of H$_2$, H$_2$-He, and H$_2$O in dynamic-DAC coupled with time-resolved X-ray diffraction and time-resolved spectroscopy

Enabling Technology Developments:

• Catching atoms in transition using dynamic-DAC and XFEL in collaboration with the LLNL and DESY groups

• Chemistry at core-electron compression using the NIF (XCHEM): NIF discovery shots scheduled in FY2021-2022
List of publications in 2019-2020


