High pressure & condensed matter research:
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- **Pressure**
  - thermodynamic property
  - properties (transport, optical, magnetic) pressure dependent
  - sometimes mimic “nano” states (high pressure form of CdS stabilized in nanometer particles)
  - dominant in determining states in planetary interiors
  - Structure of materials at high pressure & high or low temperature

- **Synchrotron Sources and Pressure**
  - Most HP experiments are brightness-limited
    - higher P implies smaller sample size
    - peak-background critical in structure determination
  - Time resolved experiments for plasticity, rheology measurements, phase transitions etc
Some of the Science Issues to Address with high pressure

- Nature of dense hydrogen - *From cryogenic to brown dwarf conditions*
- Composition, elasticity, and thermal state of Earth’s core - *Complex alloys to core P-T*
- Structures of complex hydrous phases - *Clathrates, molecular compounds, hydrous silicates,*
- Supercritical fluids and liquids - *Structure and dynamics and effect on chemical reactions*
- Structure & dynamics of silicate melts & glasses - *Implications for glass technology & volcanism*
- Planetary ices - *Structure, strength, and dynamics of ices under P, T, and stress*
- Real-time in situ monitoring of transformations in ‘real rocks” - *Modeling subduction to high P-T conditions*
- Strength and rheology of materials, including Earth materials - *Relationship to brittle and ductile failure*
- Influence of pressure and stress on magnetic properties - *From low to high temperatures*
- Dynamics of protein folding and unfolding - *Implications for food technology and life at extreme conditions*
- Structure and dynamics of nanomaterials under pressure - *Nanotubes, fullerenes, and their derivatives*
- General phase transition studies - *Mechanisms and identification with unprecedented resolution*
- Stockpile stewardship issues - *Light element studies for code verification*
**Geo- and planetary Science - Key questions**

- Earth/rocky planetary interiors
  - Stability of hydrous phases
  - How do these change elasticity/rheology?
  - Structure and chemistry of D” (Core - Mantle interface)?
  - Nature of the Core? - state of Fe, light element content
- Outer Planets
  - Gas alloy mineralogy
  - what compounds are possible at the P&T relevant to planetary interiors?

**Key parameters for interpreting Earth and planets**

- Crystal Structure
- Elastic properties
  - Simultaneous measurements at high pressure are key
- Phase relationship
- Strength and rheological properties
Crystallography: new phases at high pressure


Proposed orthorhomic structure of Fe at P/T conditions of deep Earth; impacting Geophysics, solid state physics - Andrault, Fiquet, Kunz, Visecekas, & Häusermann, Science, 278: 831 1997)

Crystallography of gas alloys

- High-Pressure Compounds in Methane-Hydrogen Mixtures: impacts planetary physics and chemistry
  Somayazulu, Finger, Hemley, Mao; Science 1996 271: 1400-1402

New High-Pressure Compounds: H$_2$-H$_2$O (X-ray structure)
- Diamond-structured clathrate
- Stable to >60 GPa
- Dense Cloud/Ice layers?

Planetary mineralogy

The nebula from which the outer planets (Saturn, Neptune and Uranus) and their satellites formed contained significant proportions of ices like ammonia, methane and water-ice. Titan is believed to have accreted from rock/ammonia monohydrate and methane hydrate. High-pressure properties in the range 0-6 GPa relevant to modeling.

Ammonia & Water: Four new phases discovered up to 6 GPa. Titan models assume negligible compression and no phase transitions. Phase VI is a simple bcc structure with substitutional site disorder of water and ammonia (Loveday & Nelmes, PRL).

Methane hydrate: Previously thought to decompose into ice and methane in the 1-2 GPa range. Two new high pressure hydrates:
- Phase II \((H_2O)_{3.5}(CH_4)\)
- Phase III \((H_2O)_2(CH_4)\)
stable to at least 10 GPa.
(Loveday and Nelmes, ISIS in collaboration with Klug and Tsi NRC)
Compression of H₂O (300 K)

- Confirmed by x-ray diffraction (bcc-like oxygen)
- No additional phases to at least 210 GPa (300 K)

Synchrotron Single Crystal X-ray Diffraction of H$_2$ and D$_2$

European Synchrotron Radiation Facility

[Loubeyre et al., Nature 383, 702(1996)]
• **Phase transitions - cross cutting topic**
  – Testing models against experimental data
  – Rigid unit modes and other computationally tractable models
    • inelastic scattering tests
    • PDFs as a test (cristobalite for example)
  – A new way of doing business
    • Measurement of phase transitions and properties simultaneously, especially under high pressure and temperature, to simulate “Earth operating conditions” (or indeed the operating conditions of any chemical system)
Cristobalite (SiO$_2$) at 300 K

Cristobalite (SiO$_2$) at 700 K

Martin Dove, Earth Sciences, Cambridge

(http://www.esc.cam.ac.uk/rums/)
Resonant Nuclear Inelastic Scattering

MOSSBAUER RESONANCE
$^{57}\text{Fe} \ 14.4 \text{ keV}$

Counts

Energy (meV)

Density of States

Energy (meV)
Second-order elastic moduli \( C_{ij} \) Singh, Mao, Shu & Hemley, Phys. Rev. Lett. 80, 2157 (1998)]; Discrepancy with theory: \( C_{44}/C_{66} = 1.70 \) (lattice strain); \( = 0.99 \) (theory)

**Plasticity of Fe and the Inner Core**
HIGH-PRESSURE X-RAY DIFFRACTION OF LIQUID IRON (ESRF)
Large volume apparatus and advantages of controllable heating at high pressure

LIQUID IRON: Pressure-Induced Coordination Changes

[Sanloup et al., Europhys.Lett., submitted]
Simultaneous structure/property measurements on unquenchable high pressure phases: Combined XRD/ultrasonics/macro-strain at NSLS, X17B1

- can not be retained to ambient P-conditions - measurement of structure/properties only while pressure is maintained
- expand to transport properties

Wollastonite CaSiO₃ at RPT

CaSiO₃ perovskite 12 GPa/1200°C

Energy disperse XRD, or monochromatic IP if required

Direct imaging of macroscopic sample strain and quality; measurement of length for ultrasonic measurements

Ultrasonic measurements

9.6 GPa 1073 K

Amplitude

Frequency (MHz)
BEYOND THE STATE OF THE ART: 300 - 500 GPa with large volume diamonds? NEW WINDOWS ON PLANETARY MATERIALS

New Diamond Anvil Cells:
LARGE VOLUME AND "3-D" ACCESS

- New ‘Transparent’ Gaskets
- Direct Measure of Stress-Strain
- New High-Pressure Probes
- Transport Measurements
- Overcome many current limitations on DAC
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