High pressure & condensed matter research:

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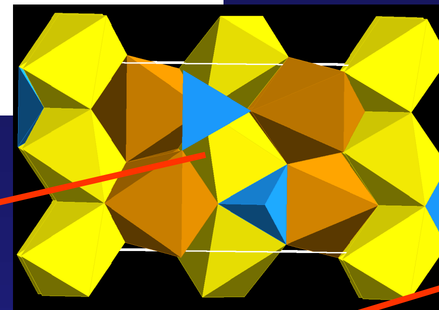
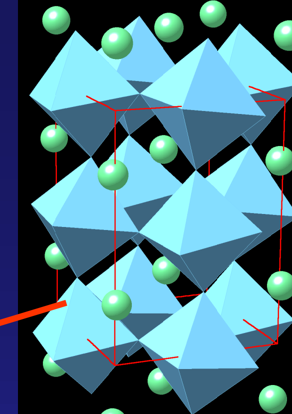
- *Pressure*
  - thermodynamic property
  - properties (transport, optical, magnetic) pressure dependent
  - sometimes mimic "nano" states (high pressure form of CdS stabilized in nanometer particles)
  - dominant in determining states in planetary interiors
  - Structure of materials at high pressure & 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

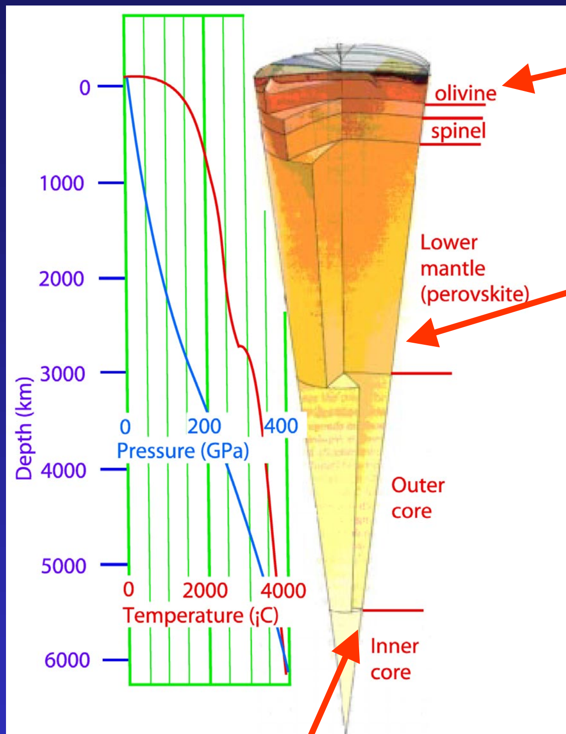
Some of the Science Issues to Address with high pressure

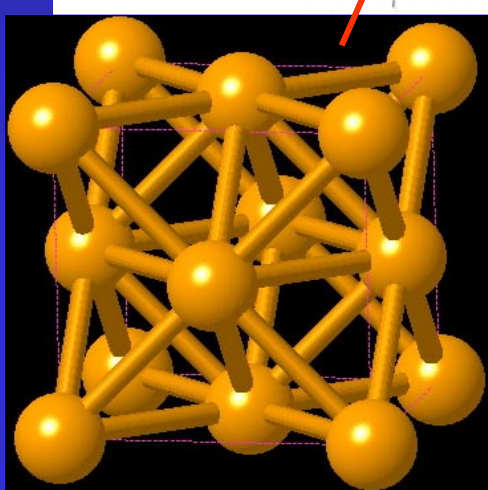
- **Nature of dense hydrogen -** ***From cryogenic to brown dwarf conditions***
- **Composition, elasticity, and thermal state of Earth's core -** ***Complex alloys to core P-T***
- **Structures of complex hydrous phases -** ***Clathrates, molecular compounds, hydrous silicates,***
- **Supercritical 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***

P/T profile of the inner Earth









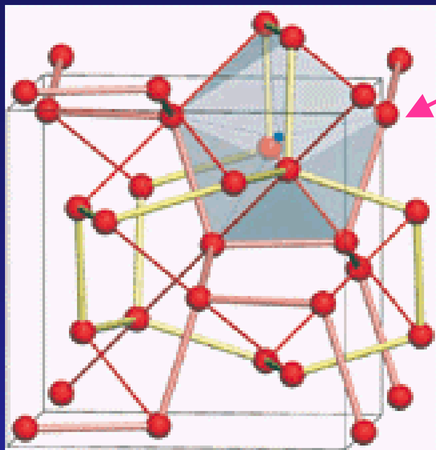
Geo- and planetary Science - Key questions

- 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

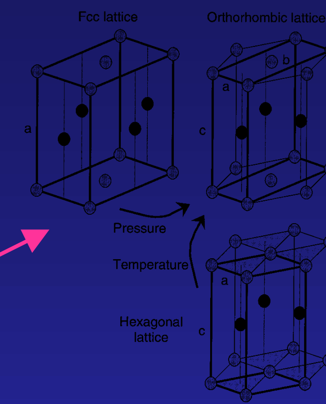
- *Crystal Structure*
- *Elastic properties*
  - *Simultaneous measurements at high pressure are key*
- *Phase relationship*
- *Strength and rheological properties*

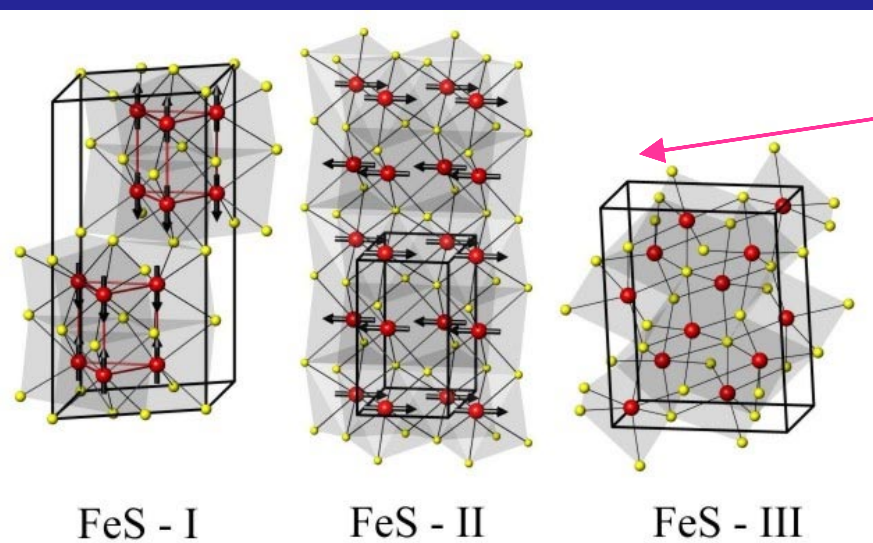
Crystallography: new phases at high pressure



Lithium becomes non-metallic at high pressure, **M. Hanfland, K. Syassen, N. E. Christensen, D. L. Novikov, Nature, 408, 174 (2000)]**

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

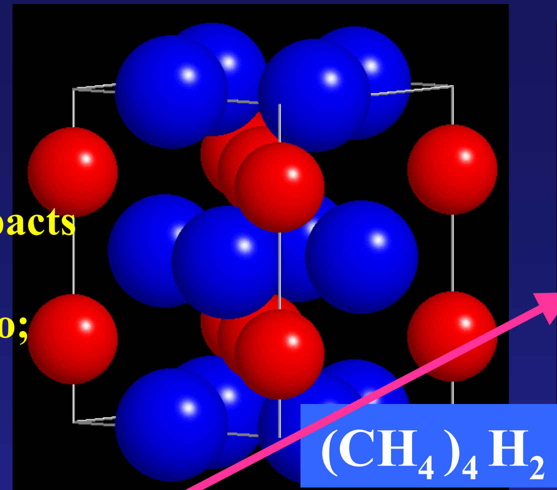


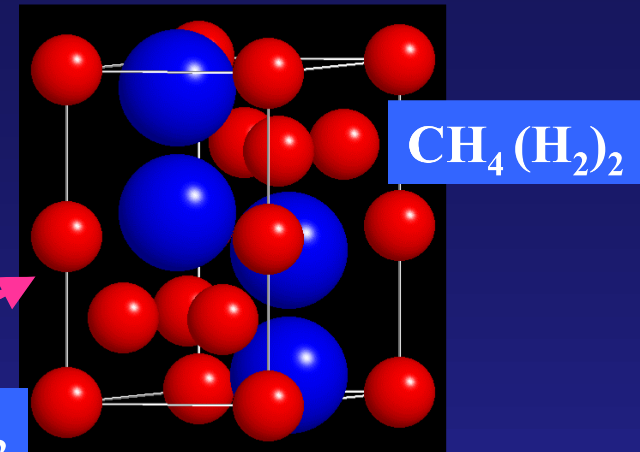


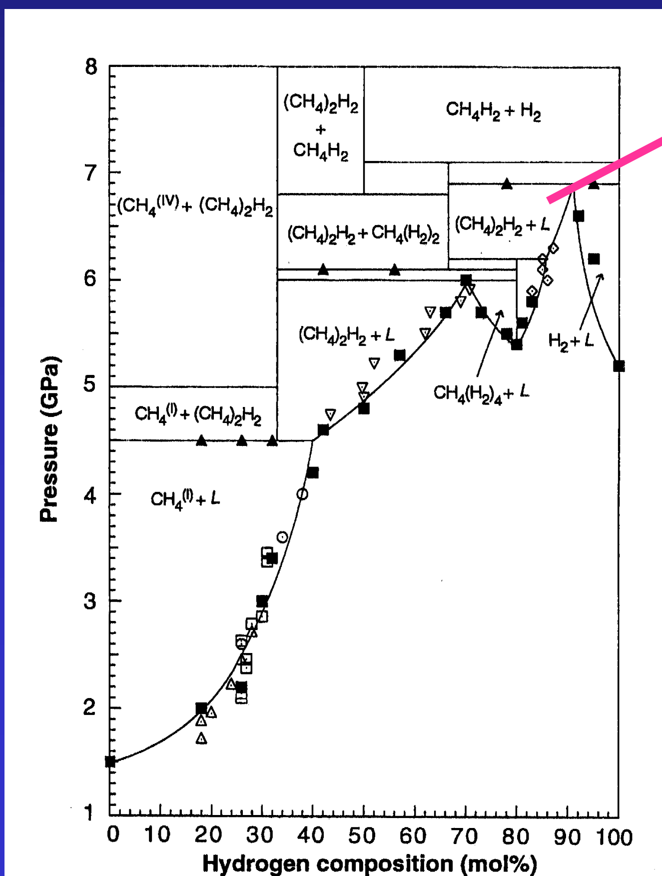
Nuclear and magnetic structure of FeS at high pressures; **Geophysics, solid state physics and chemistry; Marshall, Nelmes, Loveday, Klotz, Hamel, Besson&Parise; Phys. Rev. B 61, 11201 (2000); Nelmes, McMahon, Belmonte&Parise Phys. Rev. B 59, 9048 (1999)**

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

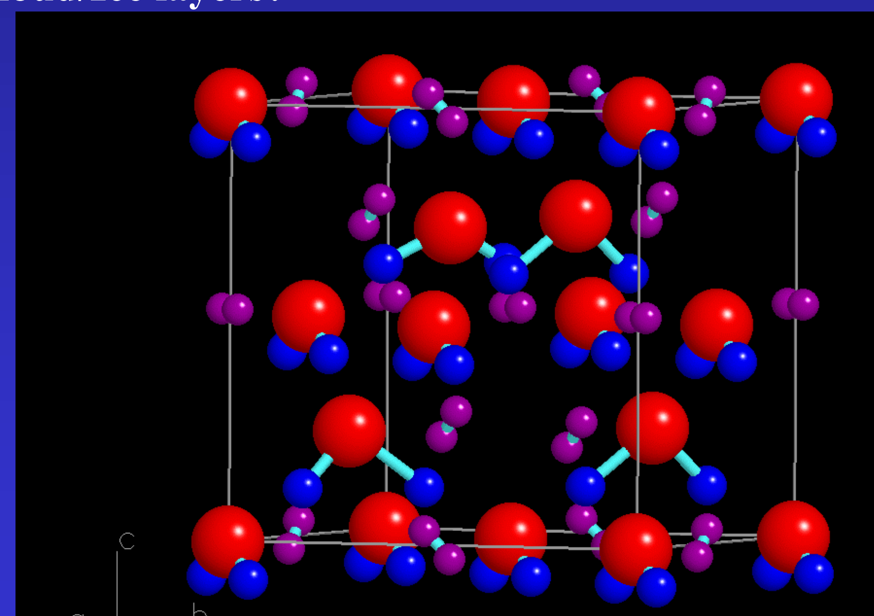






New High-Pressure Compounds: H_2-H_2O (X-ray structure

- Diamond-structured clathrate
- Stable to >60 GPa
- Dense Cloud/Ice layers?

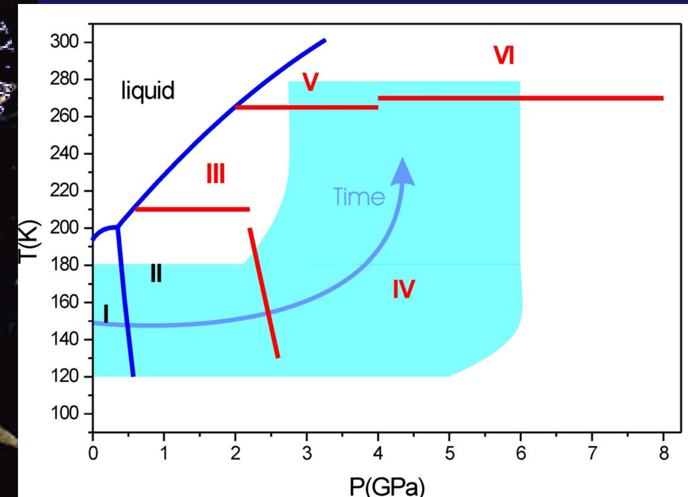


[Vos *et al*., *Phys. Rev. Lett*. 71, 3150 (1993)]

Cassini/Huygens at Titan Nov 2004

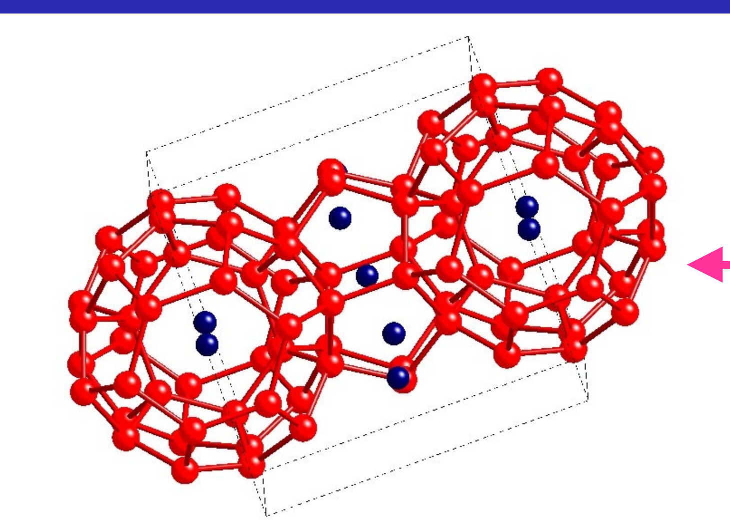
Planetary mineralogy

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

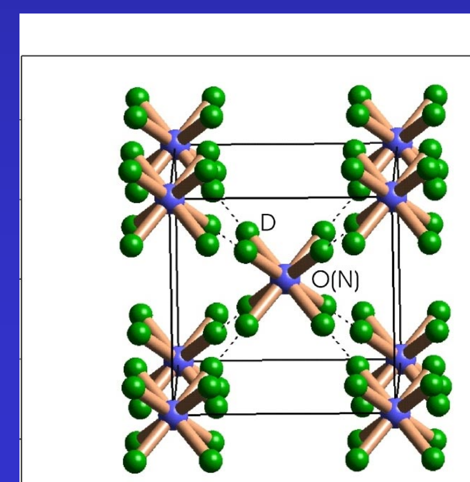
Phase VI is a simple bcc structure with substitutional site disorder of water and ammonia (Loveday & Nelmes, PRL)

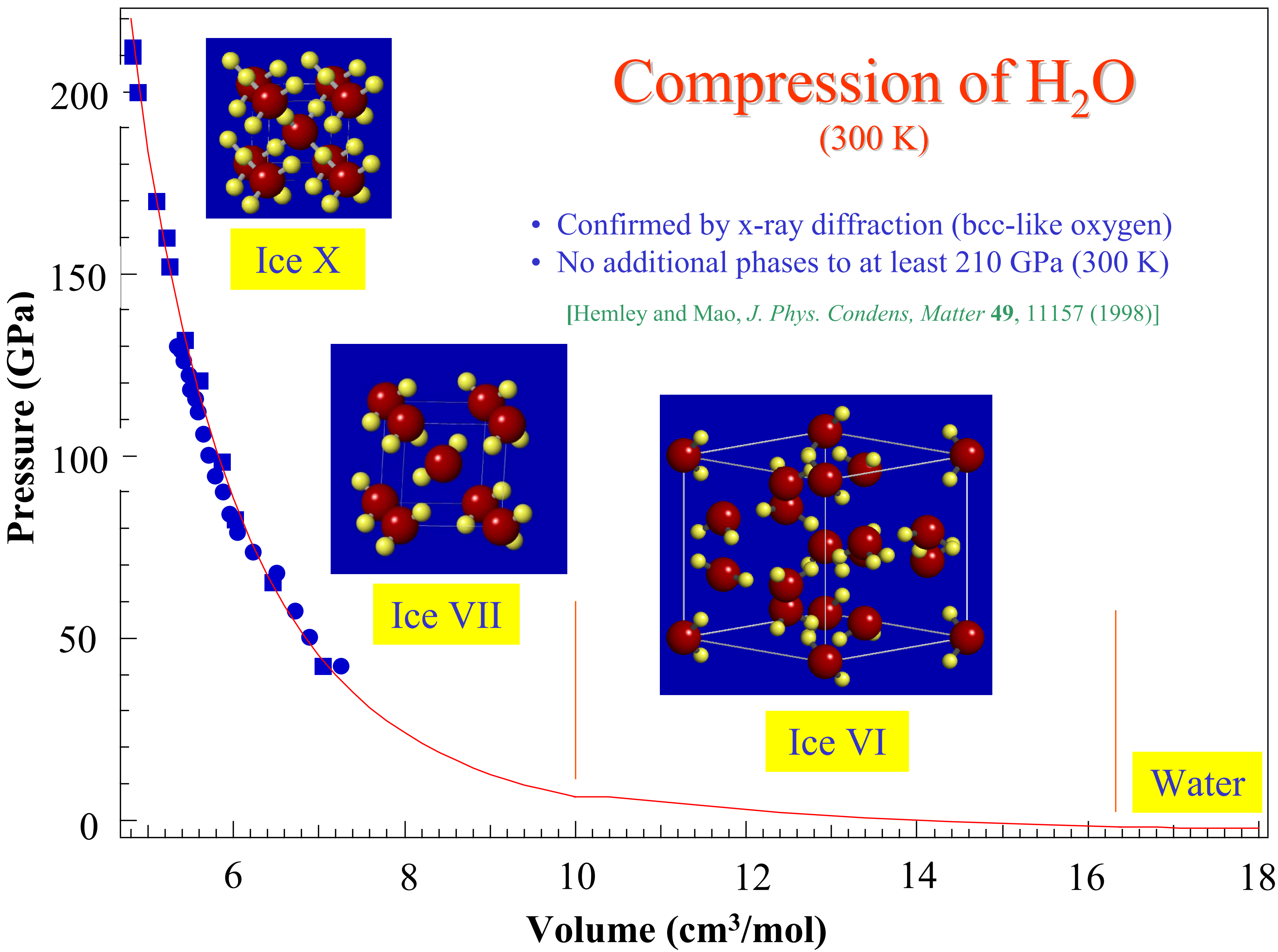


Methane hydrate: Previously thought to decompose into ice and methane in the 1-2 GPa range

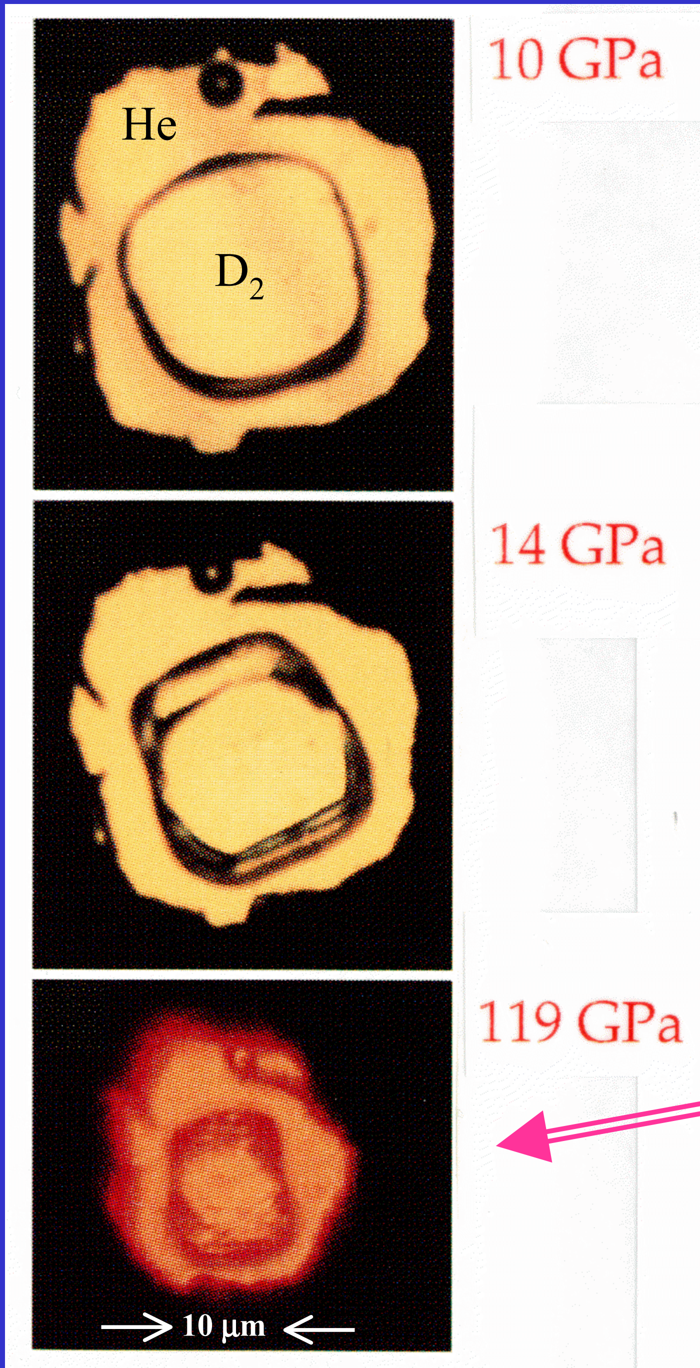
- Two new high pressure hydrates
  - phase II $(H_2O)_{3.5}(CH_4)$
  - phase III $(H_2O)_2(CH_4)$ stable to at least 10 Gpa

(Loveday and Nelmes, ISIS in collaboration with Klug and Tsi NRC



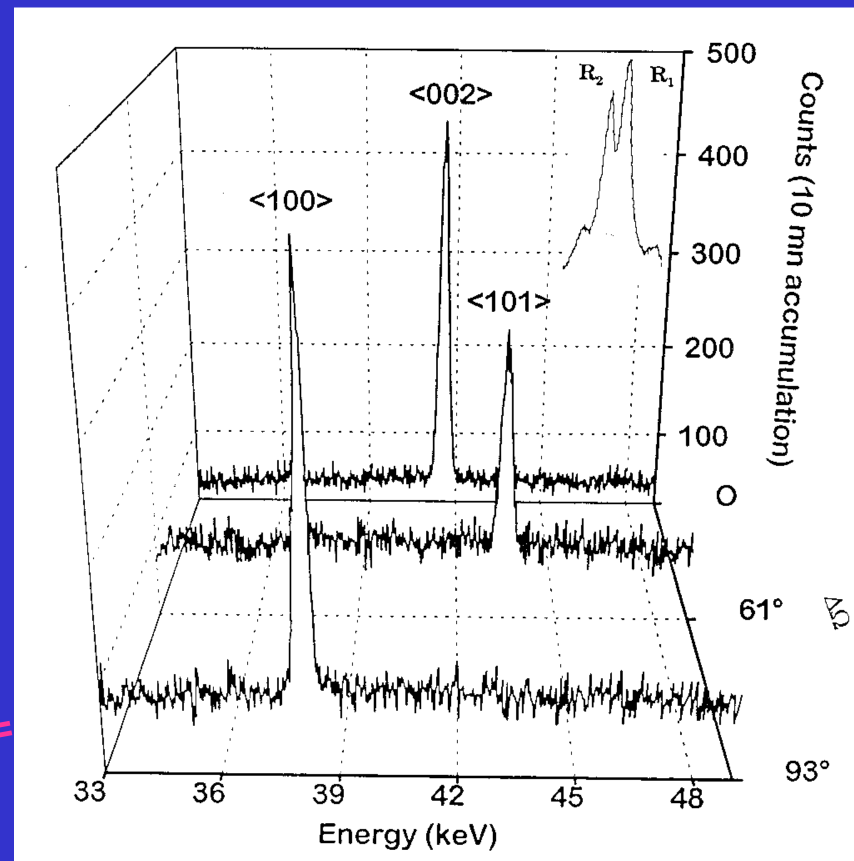


Compression of H_2O
(300 K)
• Confirmed by x-ray diffraction (bcc-like oxygen)
• No additional phases to at least 210 GPa (300 K)
[Hemley and Mao, *J. Phys. Condens, Matter* **49**, 11157 (1998)]
Ice X
Ice VII
Ice VI
Water
Pressure (GPa)
Volume (cm^3/mol)
0
50
100
150
200
6
8
10
12
14
16
18



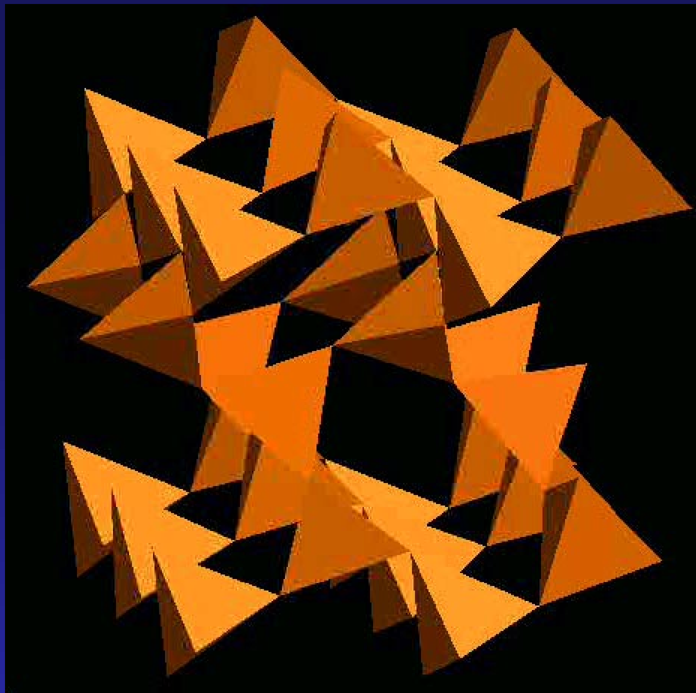
Synchrotron Single Crystal X-ray Diffraction of H_2 and D_2

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)



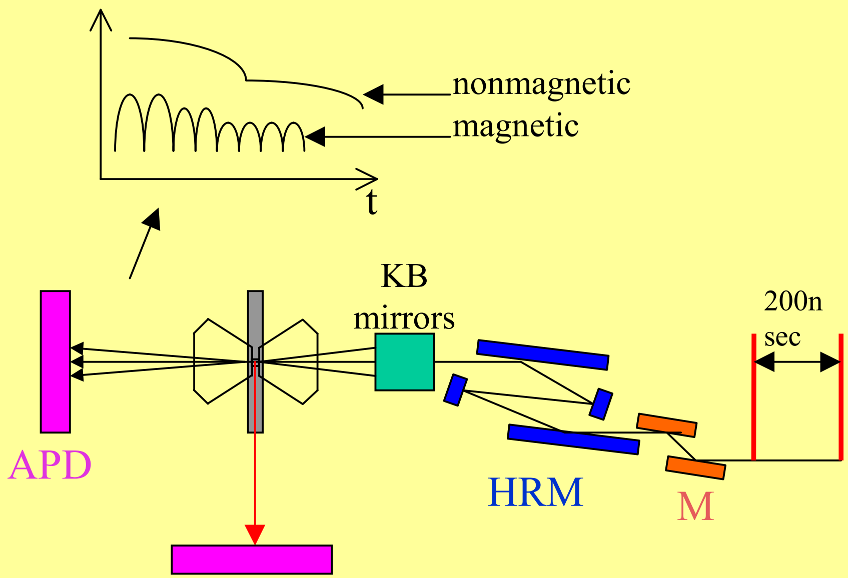
Cristobalite (SiO_2) at 300 K

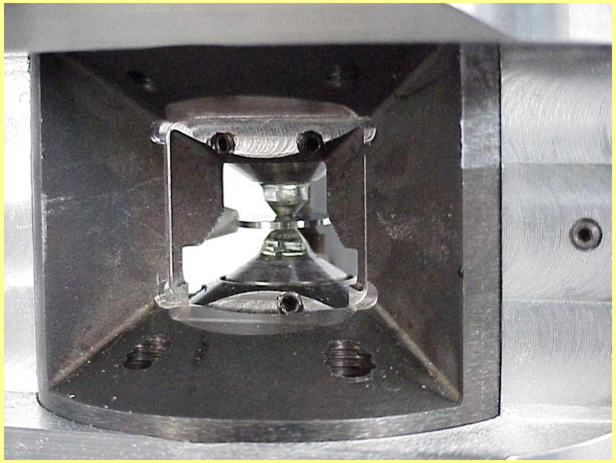
Cristobalite (SiO_2) at 700 K

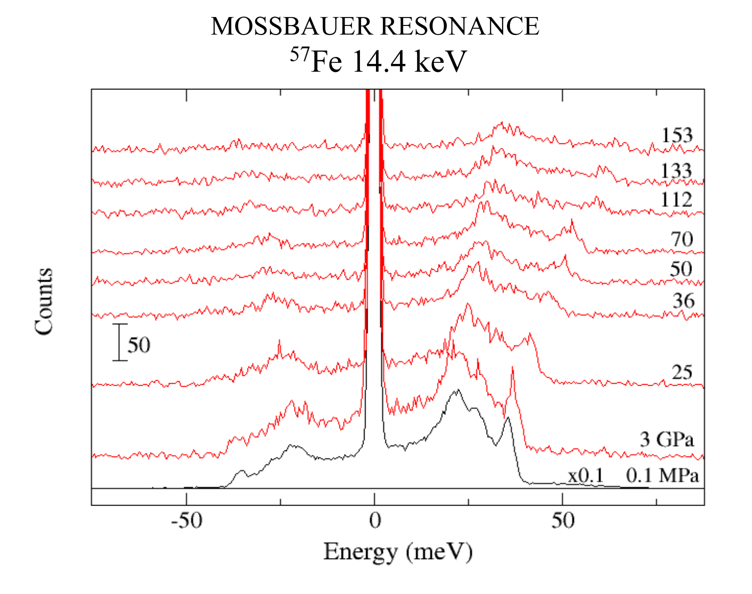
Martin Dove, Earth Sciences, Cambridge

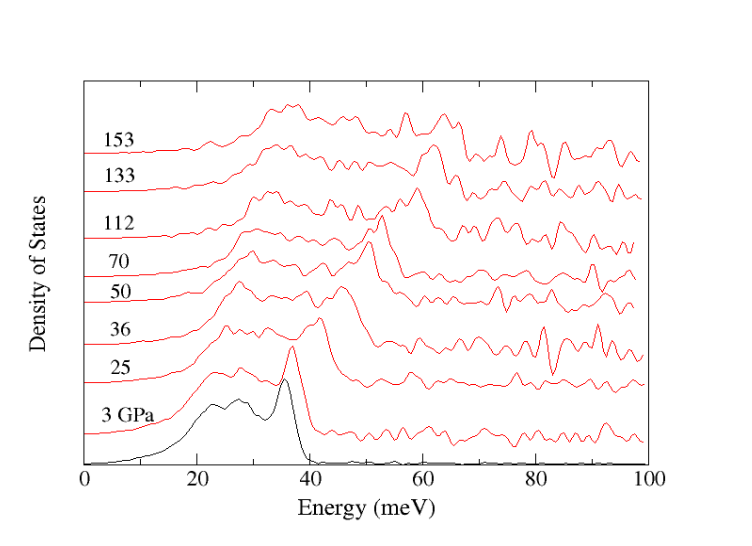
(http://www.esc.cam.ac.uk/rums/)

Resonant Nuclear Inelastic Scattering

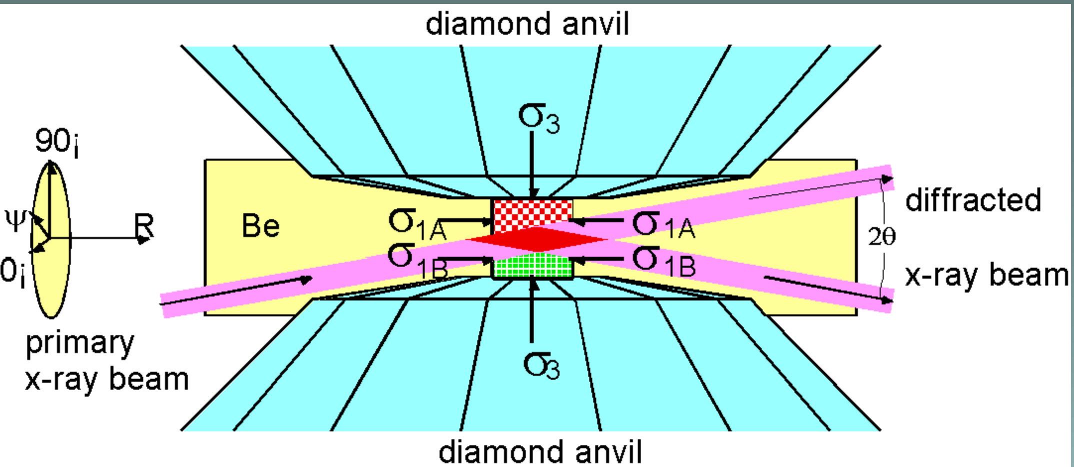


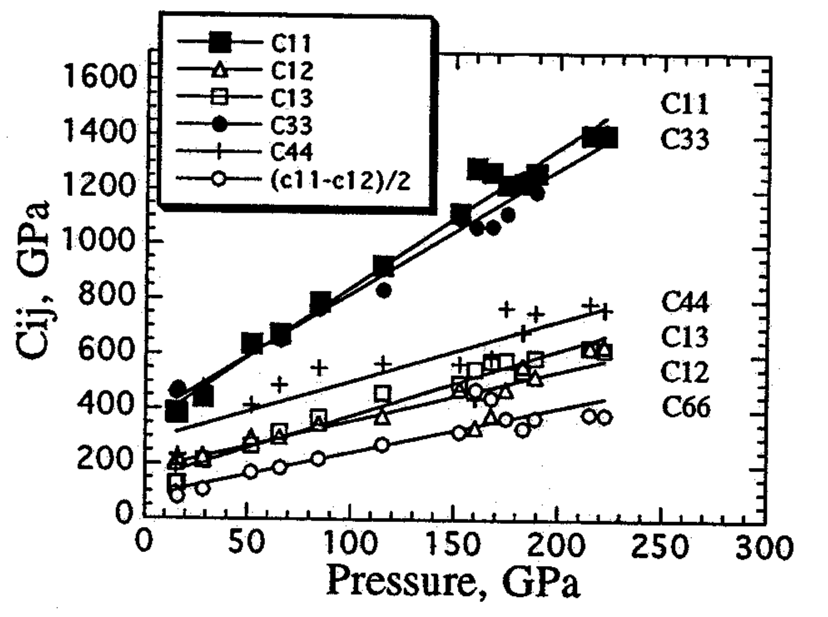






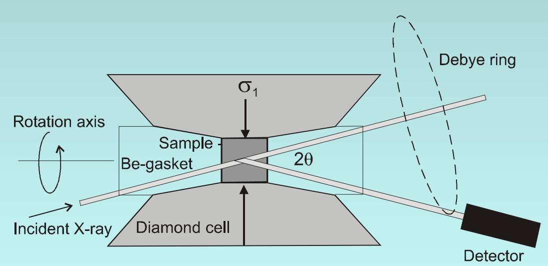
Three-Dimensional X-ray Diffraction: “X-RAY TOMOGRAPHY

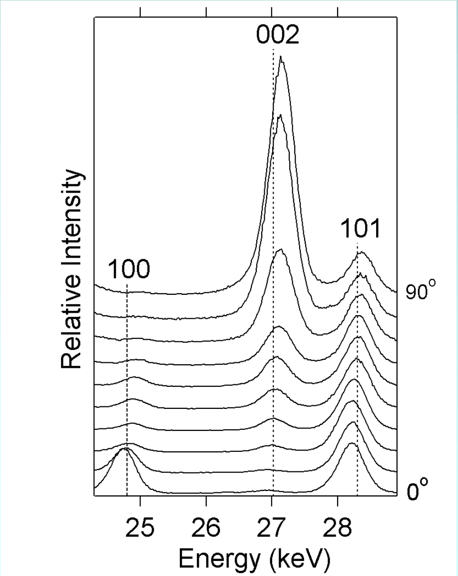


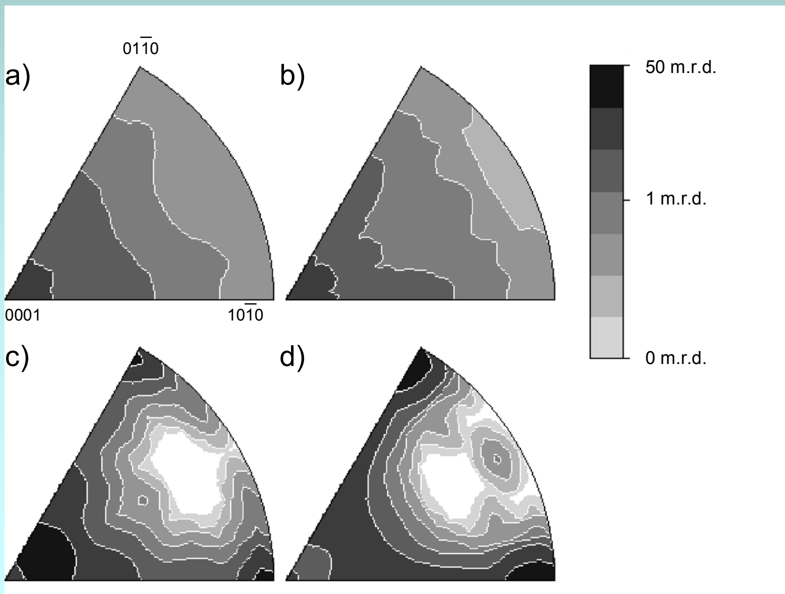


Second-order elastic moduli C_{ij} Singh, Mao, Shu & Hemley, Phys. Rev. Lett. 80, 2157 (1998)]; Discrepancy with theory: C_{44}/C_{66} = 1.70 (lattice strain); = 0.99 (theory)

Plasticity of Fe and the Inner Core

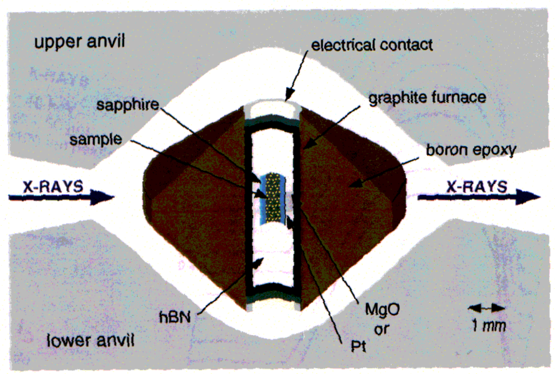


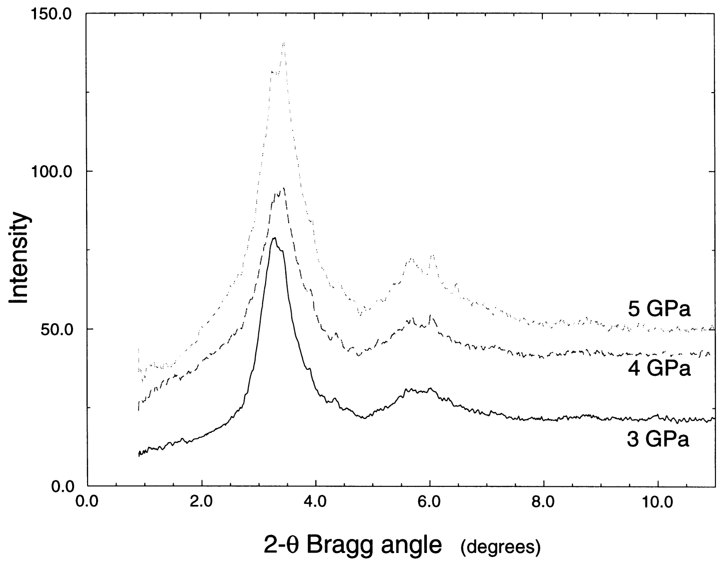




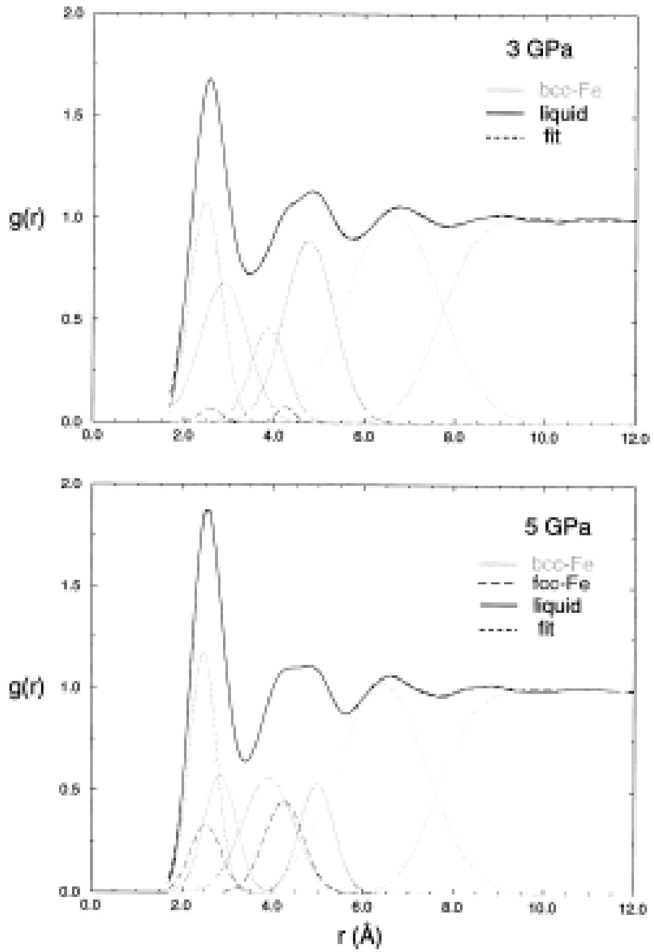
HIGH-PRESSURE X-RAY DIFFRACTION OF LIQUID IRON (ESRF)

Large volume apparatus and advantages of controllable heating at high pressure



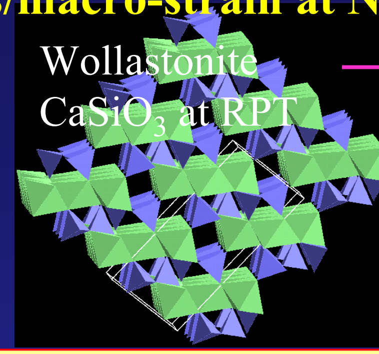


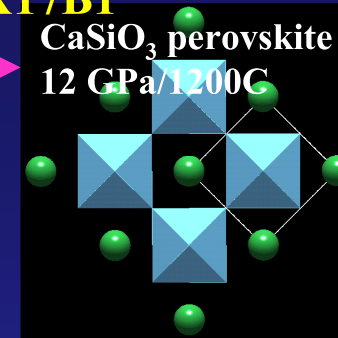
LIQUID IRON: Pressure-Induced
Coordination Changes

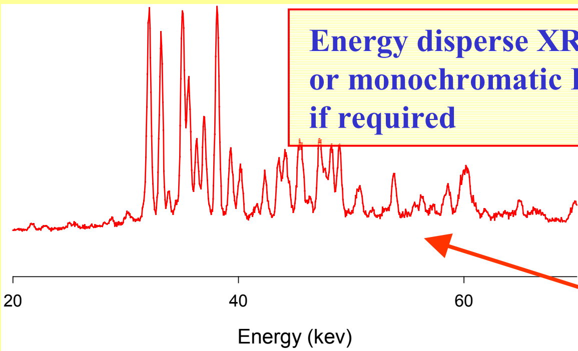


[Sanloup *et al.*, *Europhys.Lett.*, submitted]

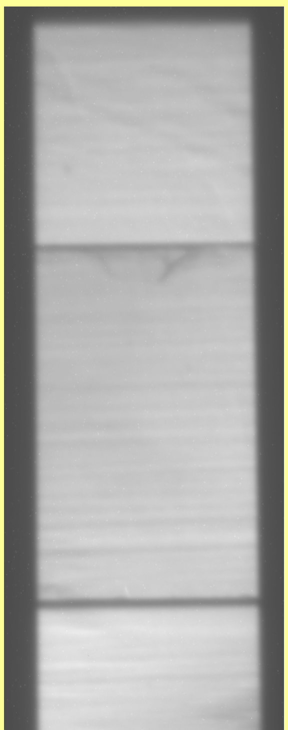
Simultaneous structure/property measurements on *unquenchable* high pressure phases: Combined XRD/ultrasonics/macro-strain at NSLS, X17B1

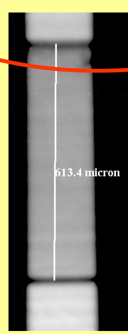




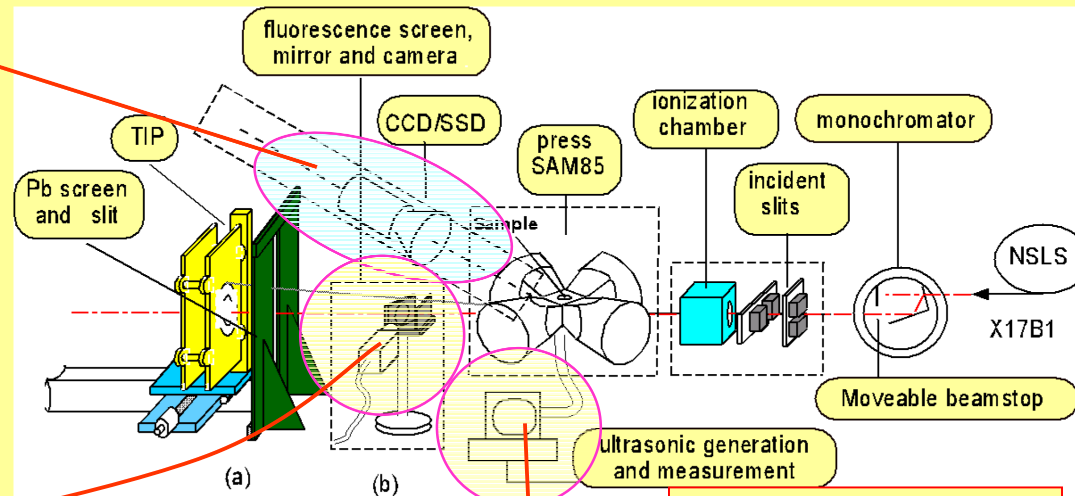


Energy disperse XRD, or monochromatic IP if required

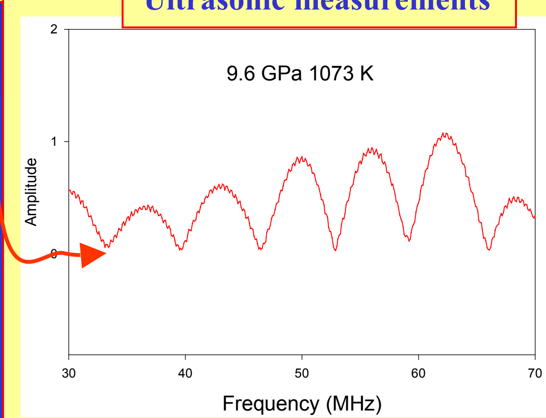




Direct imaging of macroscopic sample strain and quality; measurement of length for ultrasonic measurements



Ultrasonic measurements

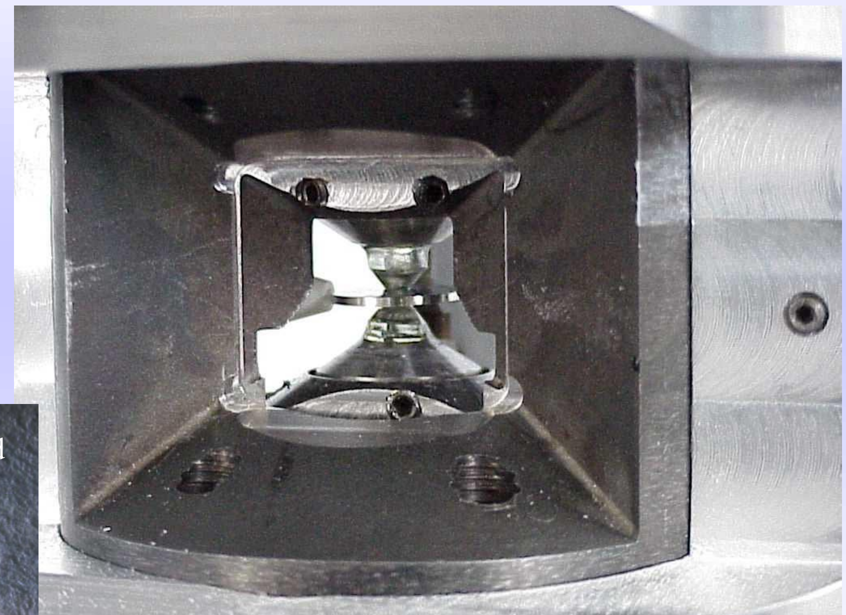


- *can not* be retained to ambient P-conditions - measurement of structure/properties ***only while pressure is maintained***
- ***expand to transport properties***

BEYOND THE SATE 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


IN GOD WE TRUST
LIBERTY

Acknowledgements

- NSF-DMR, ACS-PRF
- CHiPR group (DJ Weidner, RC Liebermann, B. Lee @ Stony Brook; Jian Xu, Y. Fei, CT Prewitt @ GPL) Paris/Edinburgh group (R. Nelmes, M. Besson, JS Loveday, M. McMahon) - Edinburgh/ISIS/Daresbury
- David Keen, W. Marshall (ISIS)
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