Science-based Session

What breakthroughs can 1 nm probe and 0.1 meV resolution bring to:

- High Pressure Sciences
  - *X17 at NSLS*
  - *HPCAT at APS*

- Earth Sciences
  - *X1A , X17, X26 at NSLS*
  - *GSECARS at APS*

How do we make this happen?

Dedicated beamlines?

Infrastructure?

Nanoprobes for Earth sciences

- Soft rock

  Biogeology, biogeochemistry, micro-nano-paleontology

  Origin of life, forensic in Jurassic...

  Astrobiology

  Environmental geology, global change

- Hard rock

  Nano-mineralogy

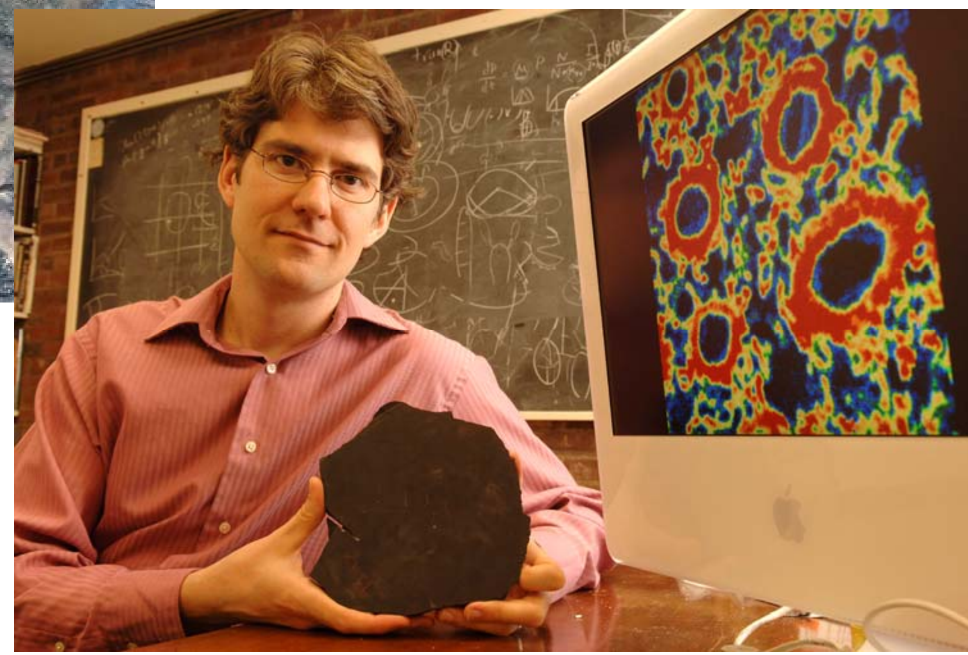
  Nano-petrology

- Deep Earth

  Upper mantle, transition zone, lower mantle, CMB,
  outer core, IOB, inner core

  Hydrology cycle, carbon cycle,volatile cycle, ...

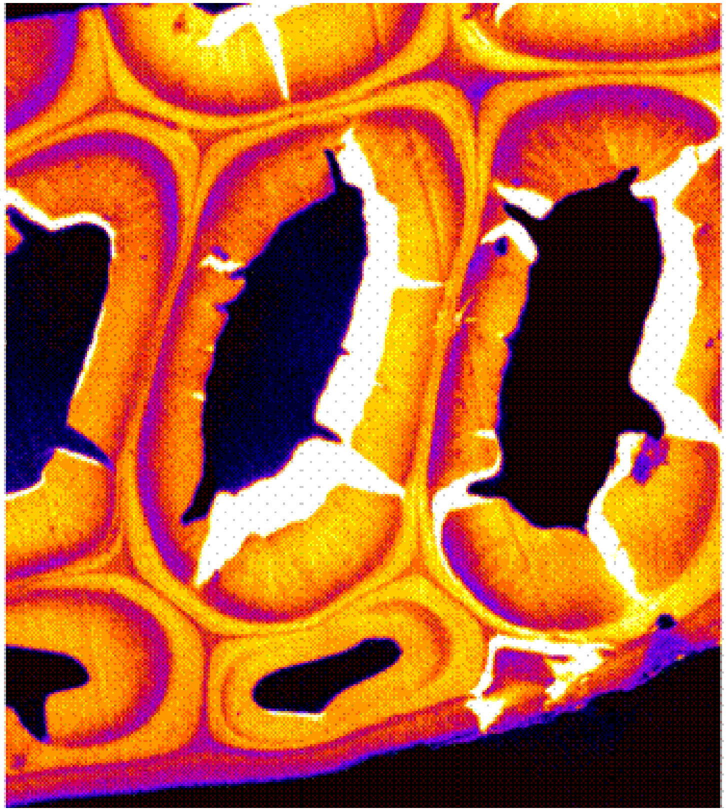
Prehistoric Mystery Organism Verified as Giant Fungus

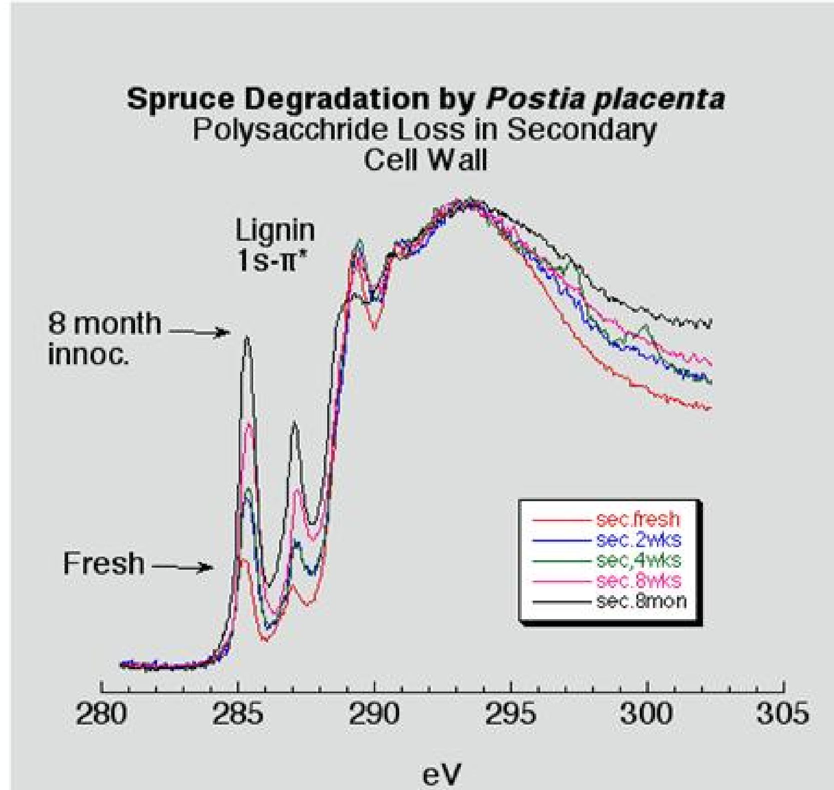


C. Kevin Boyce, Fran Hueber, Carol Hotton, Marilyn Fogel, George Cody, and Robert Hazen, in *Geology,* 22 May 2007

National Museum of Natural History., "the weirdest organism that ever lived."

Synchrotron Based Scanning Transmission X-ray Microscopy and Microspectroscopy (C-, N-, O-XANES)



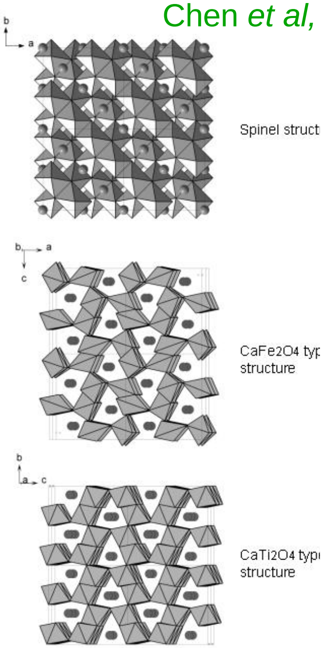


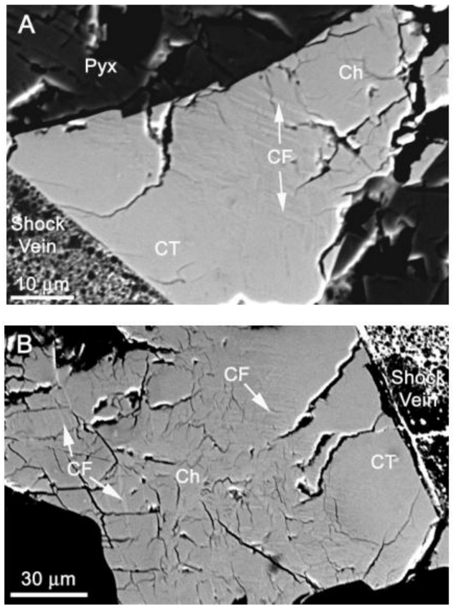
This awesome image is of compression wood from red spruce. Note that the darker (purple) regions correspond to increased lignin content. This image shows that in compression wood lignin accumulates in the secondary cell wall next to the primary cell wall at concentrations as high as observed in the compound middle lamellae. The finest scale features in this image are on the order of 50 nm. -- George Cody

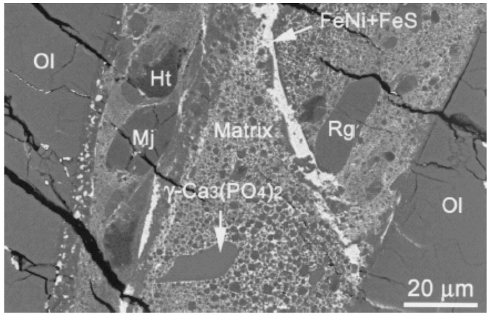
Pressure changes mineralogy and petrology-- Examples: Ultrahigh-pressure metamorphism and meteorite impact metamorphism

Discovery of two new minerals, HP forms of chromite, in shocked Suizhow Meteorite (China)

Chen *et al, PNAS* (2003)



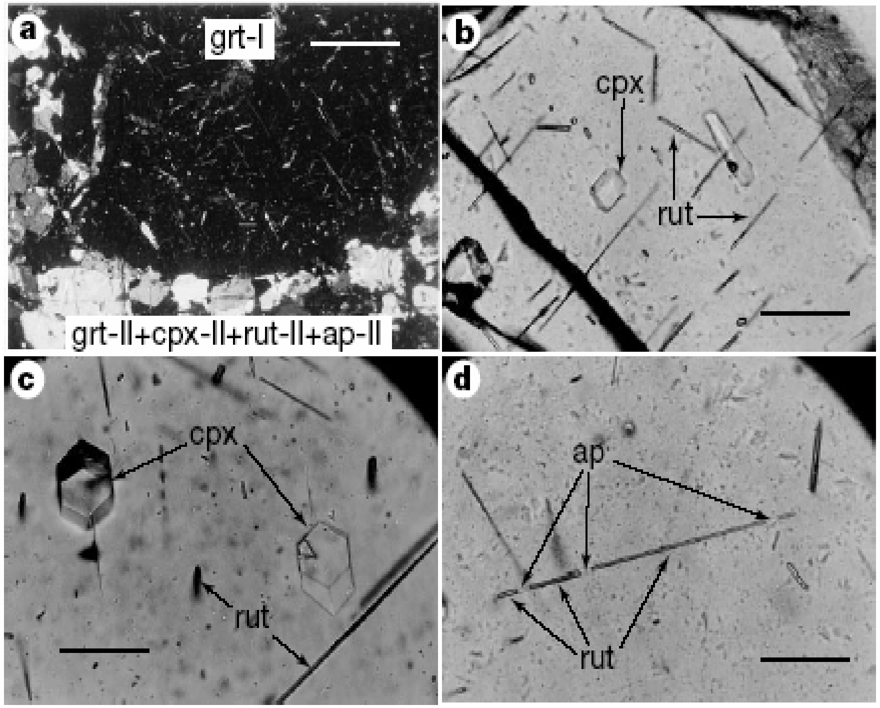




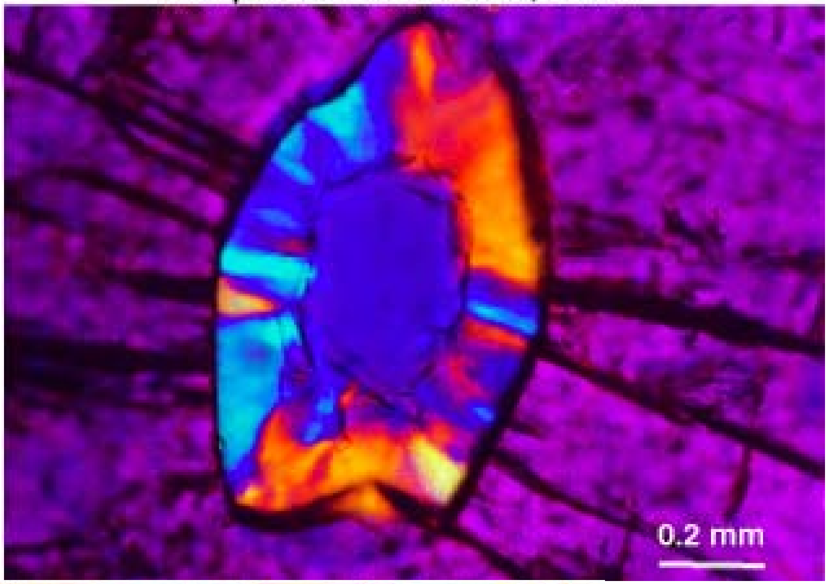
New mineral, Tuite, in shocked meteorite

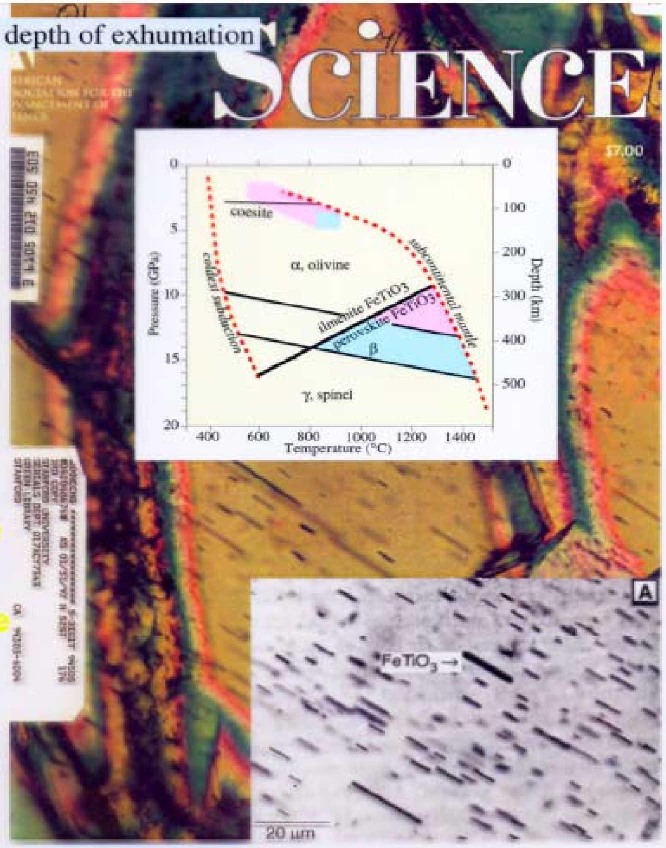
Xie *et al, GCA* (2002)

Micro-mineral exsolutions in eclogite from Sulu ultrahigh pressure metamorphic belt (China)



Ye, Cong, & Ye, *Nature* (2000)

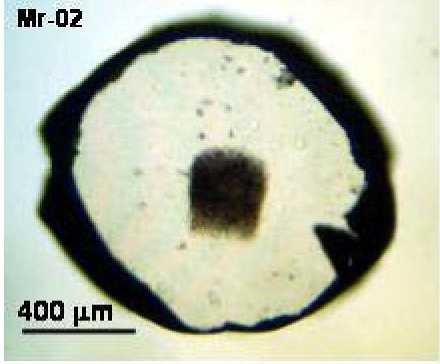


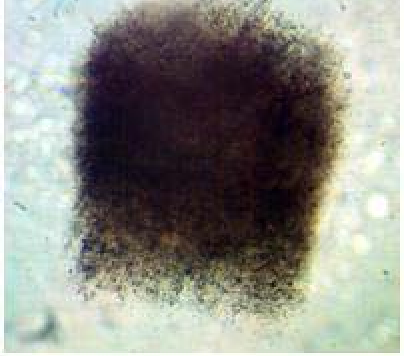


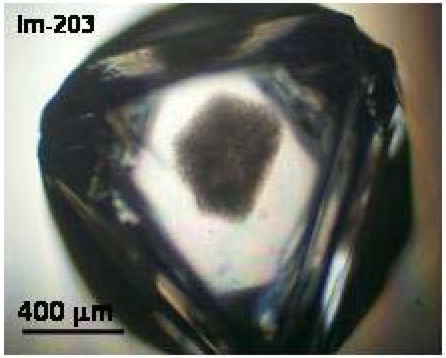
Coesite

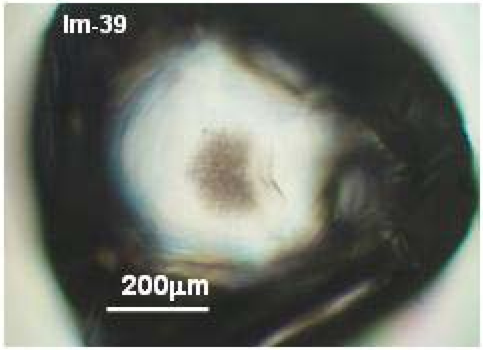
Ultrahigh pressure metamorphic petroloby

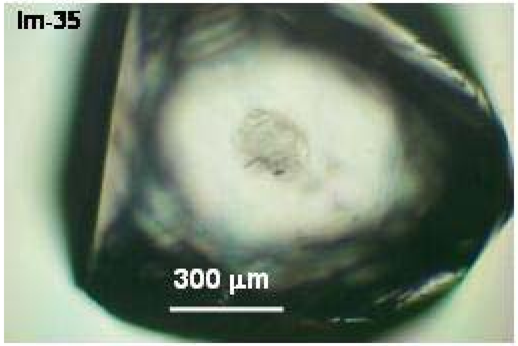
Micro-nano spinels in olivine

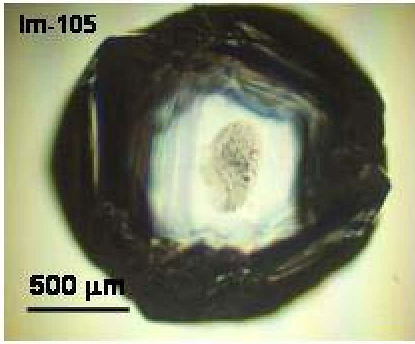




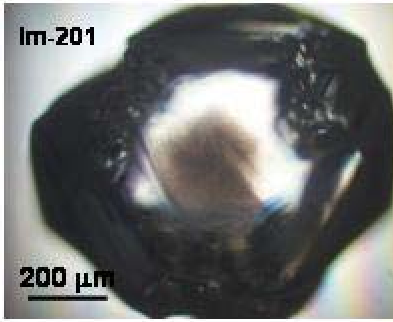


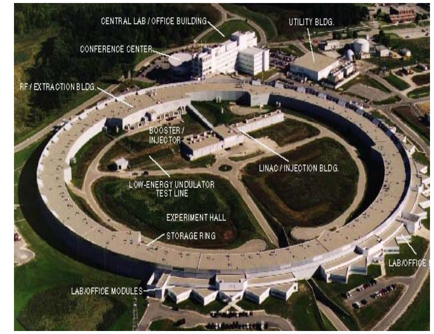






Mineral & fluid inclusions in diamonds



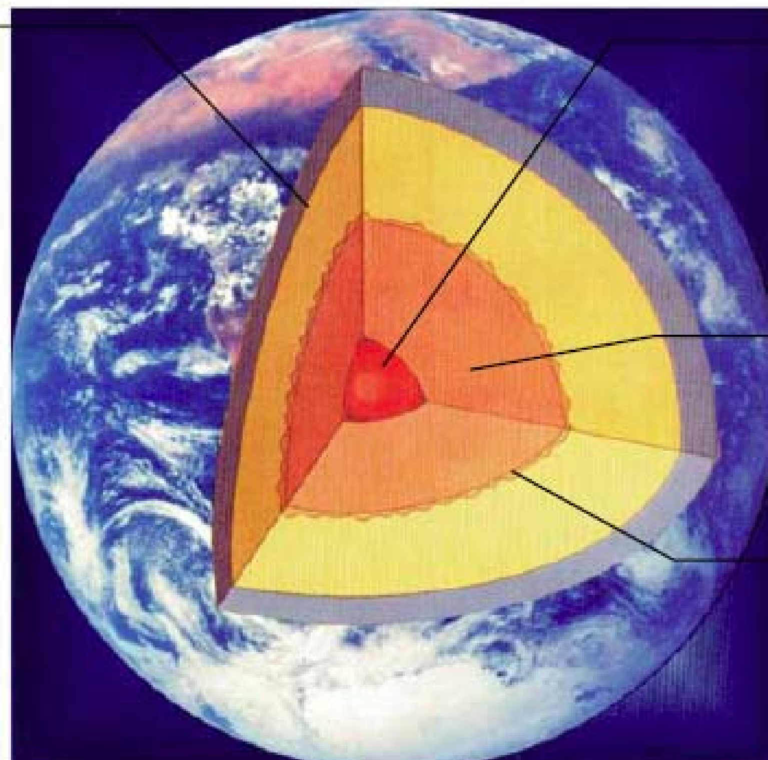


- Geophysical observations
- High P-T experiments
- Materials properties

Models & Interpretations

Deep Earth Studies

Mantle dynamics?
Discontinuity?
Phase transitions?
Element partitioning?
Melting?
Oxidation?
Hydration?
High-low spin?
Temperature?
Composition?



Inner core anisotropy?
Super-rotation?
Magnetism?

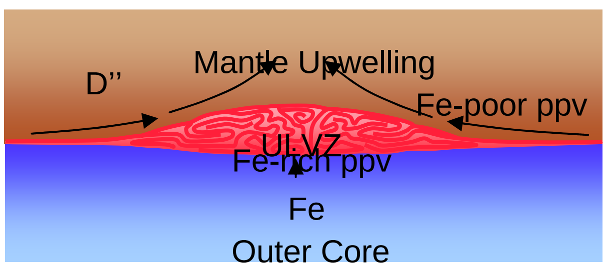
Core dynamo?
Composition?
Temperature?

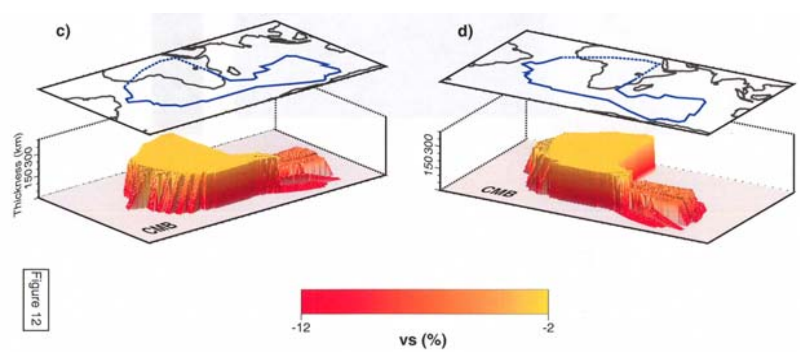
CMB reactions?
Partitioning?
Anisotropy?
Melting?

Pressure dictates deep Earth properties

D" layer at core-mantle boundary

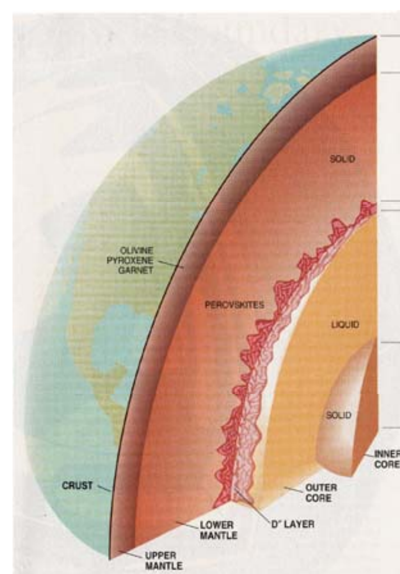
- Discovery of post-perovskite [Murakami et al *Science* (2004), Oganov et al *Nature* (2004)]
- Fe-rich ppv [Mao et al *PNAS* (2004, 2005)]
- Very low Vs and Vp in Fe-rich ppv for ULVZ [Mao et al *Science* (2006)]
- Shear-wave splitting [Merkel et al *Science* (2006)]
- Discontinuity at the top of D" [Lin et al *Nature* (2005)]





High-*P* iron in the core and mantle

- High *P-T* Birch's Law of Fe[Lin et al *Science* (2005)]
- Fe melting Nguyen & Holmes Nature (2004)]
- High-spin-low-spin transitions of Fe [Badro et al *Science* (2003; 2004)]
- Seismic velocity of Fe [Mao *et al Science* (2002); Fiquet *et al Science* (2002)]
- Fe-Si alloys in the core [Lin *et al Science* (2002)]



New sciences appears across the board at each *P* interval

- Geophysics & Geochemistry

  In situ measurements from crust to core conditions
- Biology & Biochemistry

  Origin and evolution of life
- Fundamental Chemistry

  New Periodic Table and bonding
- Fundamental Physics

  Novel transitions and novel states of matter
- Materials Science

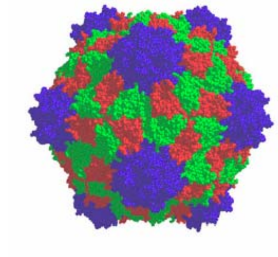
  Electronic materials *Magnetic materials*
  Superhard materials *Optical materials*
  Biological materials *Nanomaterials*
  Energetic materials (hydrogen storage)

  High *P-T* exploration for ambient *P* applications

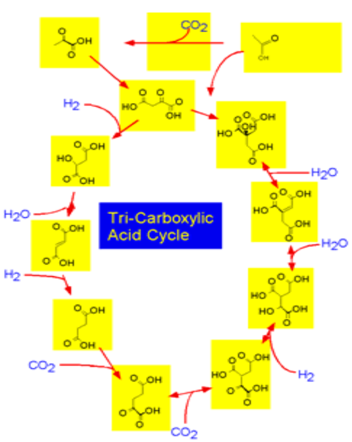
Pressure change biomaterials -- Examples: bacteria and virus

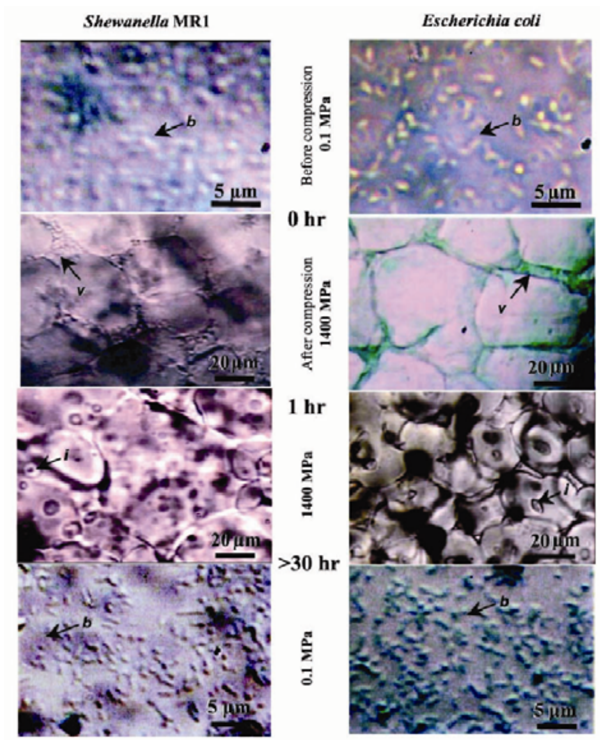
- BIOCHEMICAL REACTIONS IN HYDROTHERMA FLUIDS

- LIFE IN EXTREME ENVIRONMENTS (>1600 MPa)

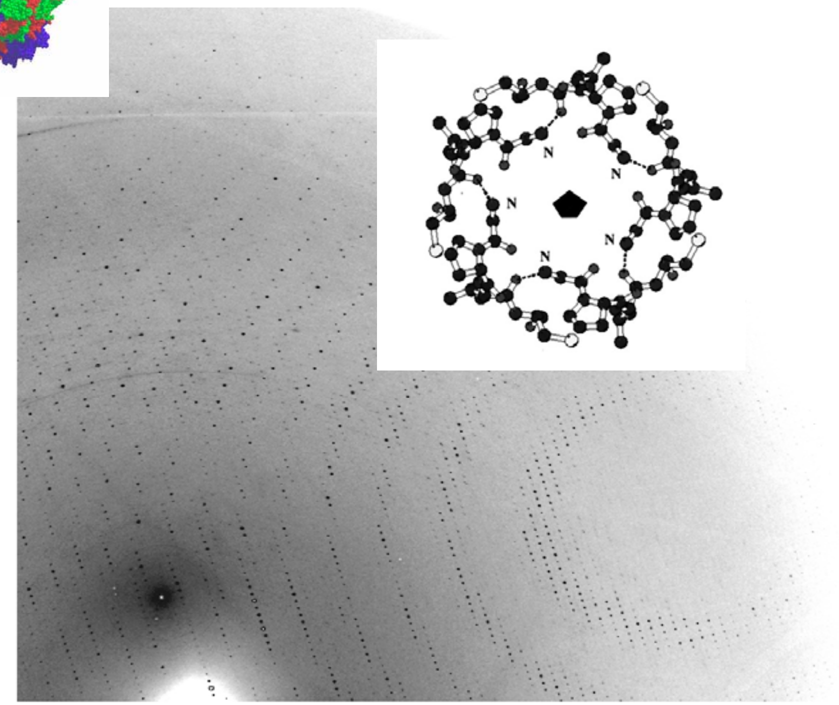


Single-Crystal Diffraction of Cow Pea Mosaic Virus





[Sharma *et al*., *Science* ***295***, 1514 (2002)]



3.5 kbar

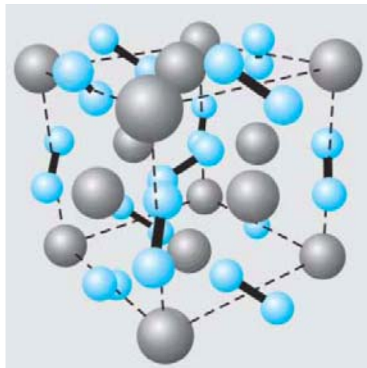
[Lin *et al*., *Acta Crystal.* ***D61***, 737 (2005)]

- PRESSURE EFFECTS ON STRUCTURE-FUNCTION RELATIONS

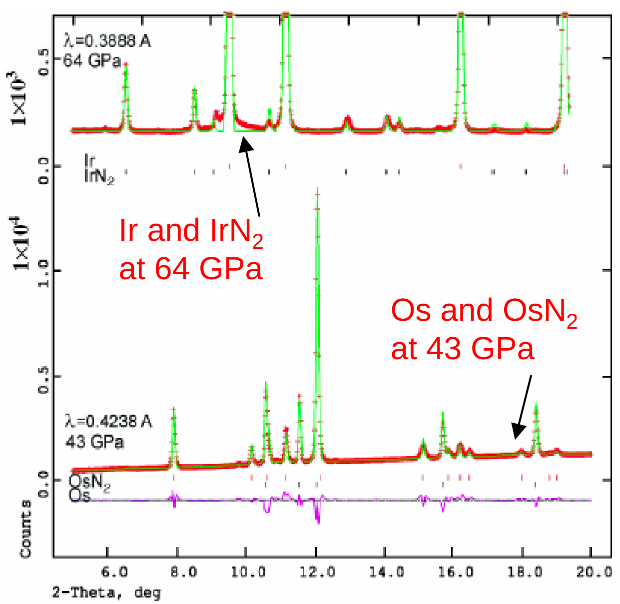
Pressure changes chemistry -- Example: nitrogen and nitrides

Noble metals (Pt, Ir, Os) form new class of nitrides at high pressures

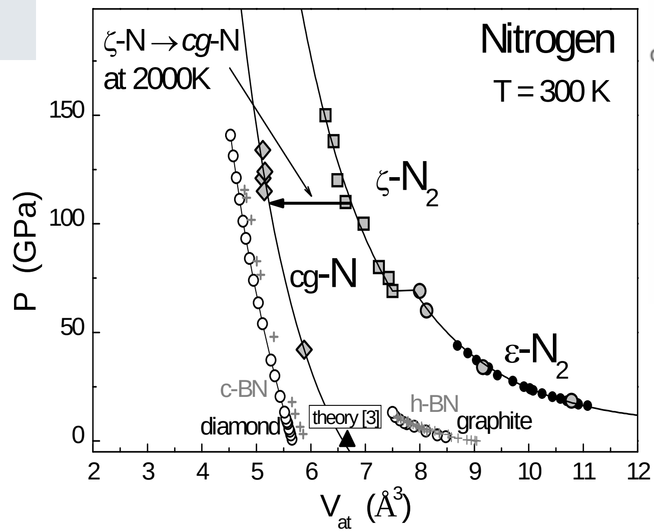
Degtyareva et al, *Nature Mat*. (2005); Crowhurst *et al, Science* (2006); Young *et al, PRL* (2006)



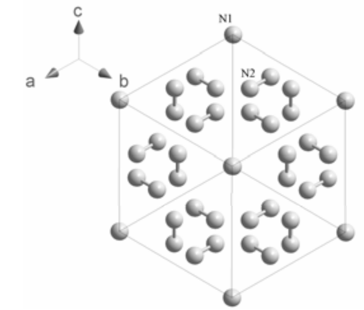
PtN$_2$ in pyrite structure



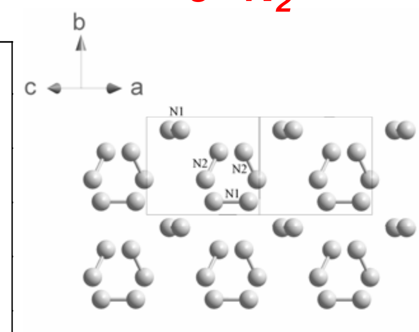
X-ray diffraction measurements reveal the structure of framework "polymeric" nitrogen



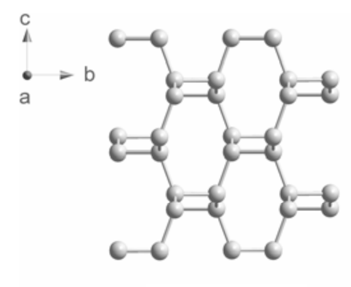
Eremets *et al*, *Nature Mat.* (2004); Goncharov *et al, PRL* (2000); Eremets *et al, Nature* (2001)



ε - N$_2$



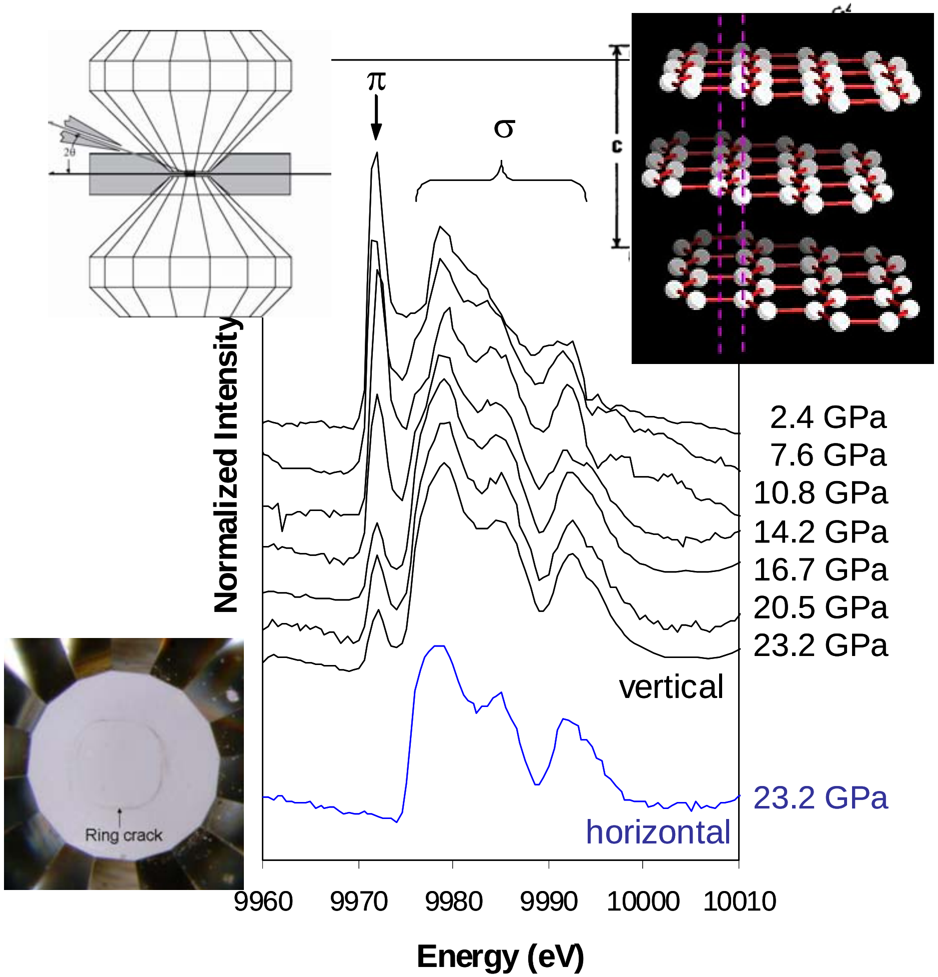
ζ - N$_2$



cg - N

Pressure changes chemical bonding– Example: high-pressure synchrotron x-ray K-edge spectroscopy of light elements

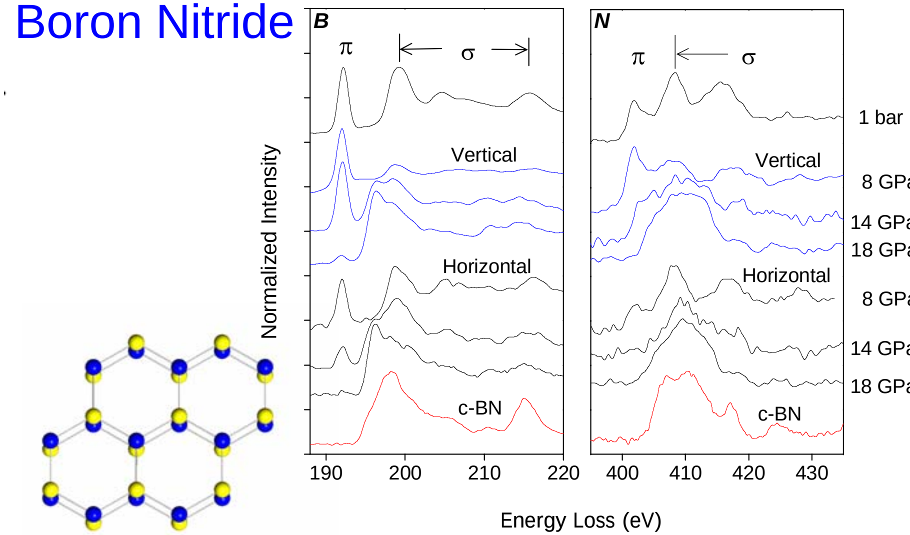
Bonding changes in superhard graphite



X-ray raman of graphite at high pressure showing the evolution of bonding and transformation to a new, superhard phase

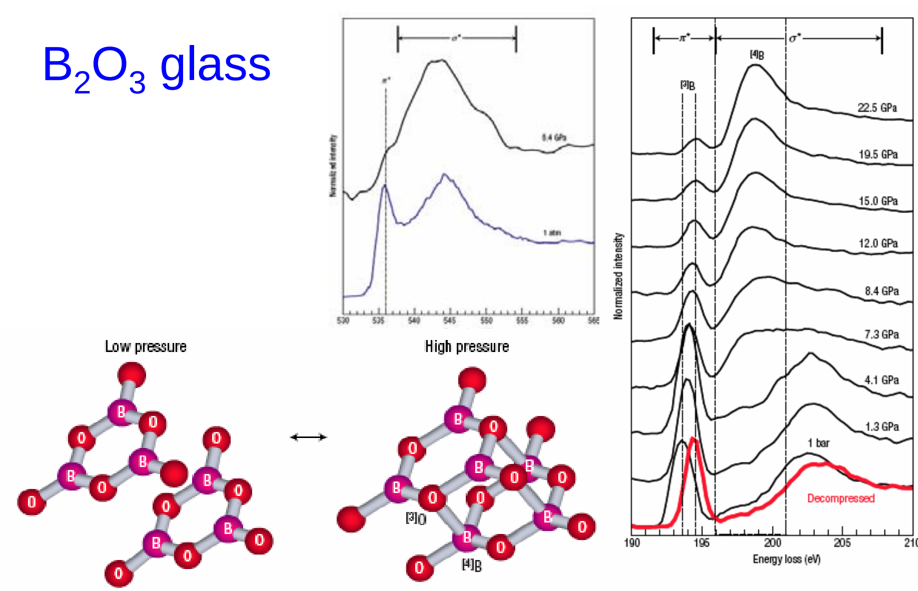
W. Mao *et al, Science* (2003)

Boron Nitride



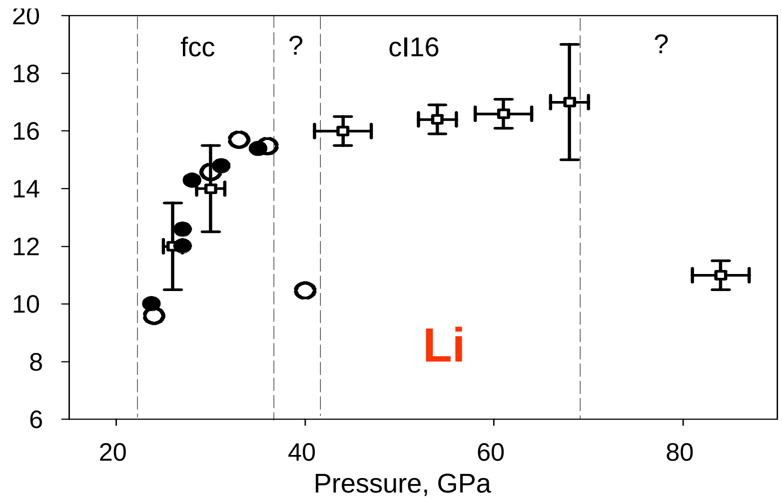
Meng *et al*, *Nature Mat.*(2004)

B_2O_3 glass



Lee *et al*, *Nature Mat.*(2005)

Pressure changes electronic structures --
Example: novel superconductivity in light elements

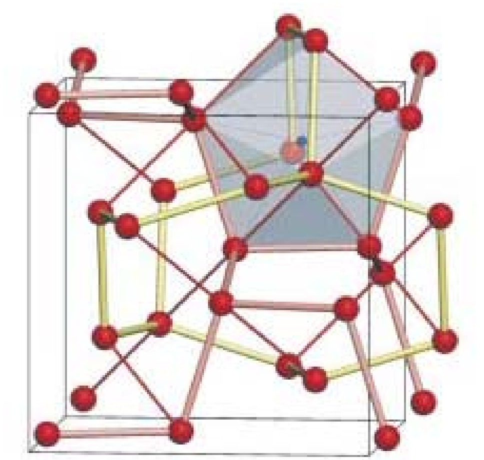


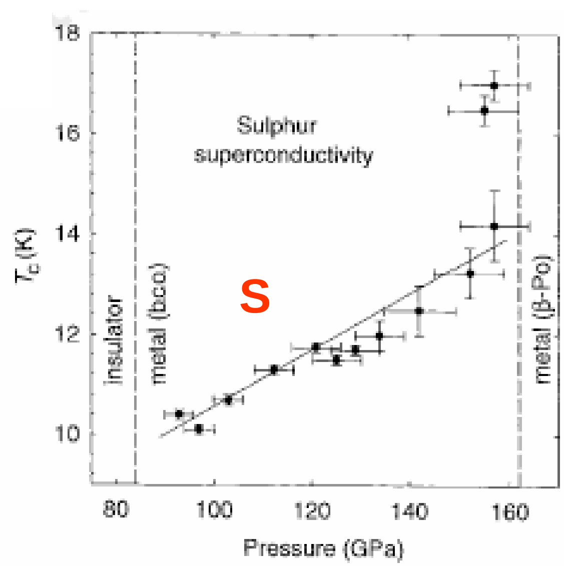
Shimizu *et al, Nature* (2002)
Struzhkin *et al, Science* (2002)
Hanfland *et al, Nature* (2000)
Neaton & Ashcroft *Nature* (1999)

-NOVEL SUPERCONDUCTORS -- O, S, B, Fe, Li, C…

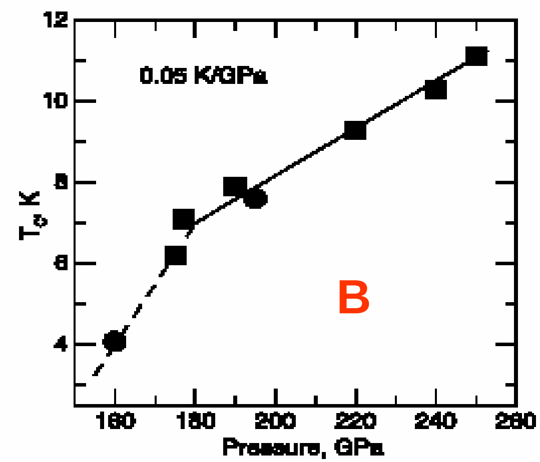
New Periodic Table of Superconductors

Ashcroft, *Nature* (2002)



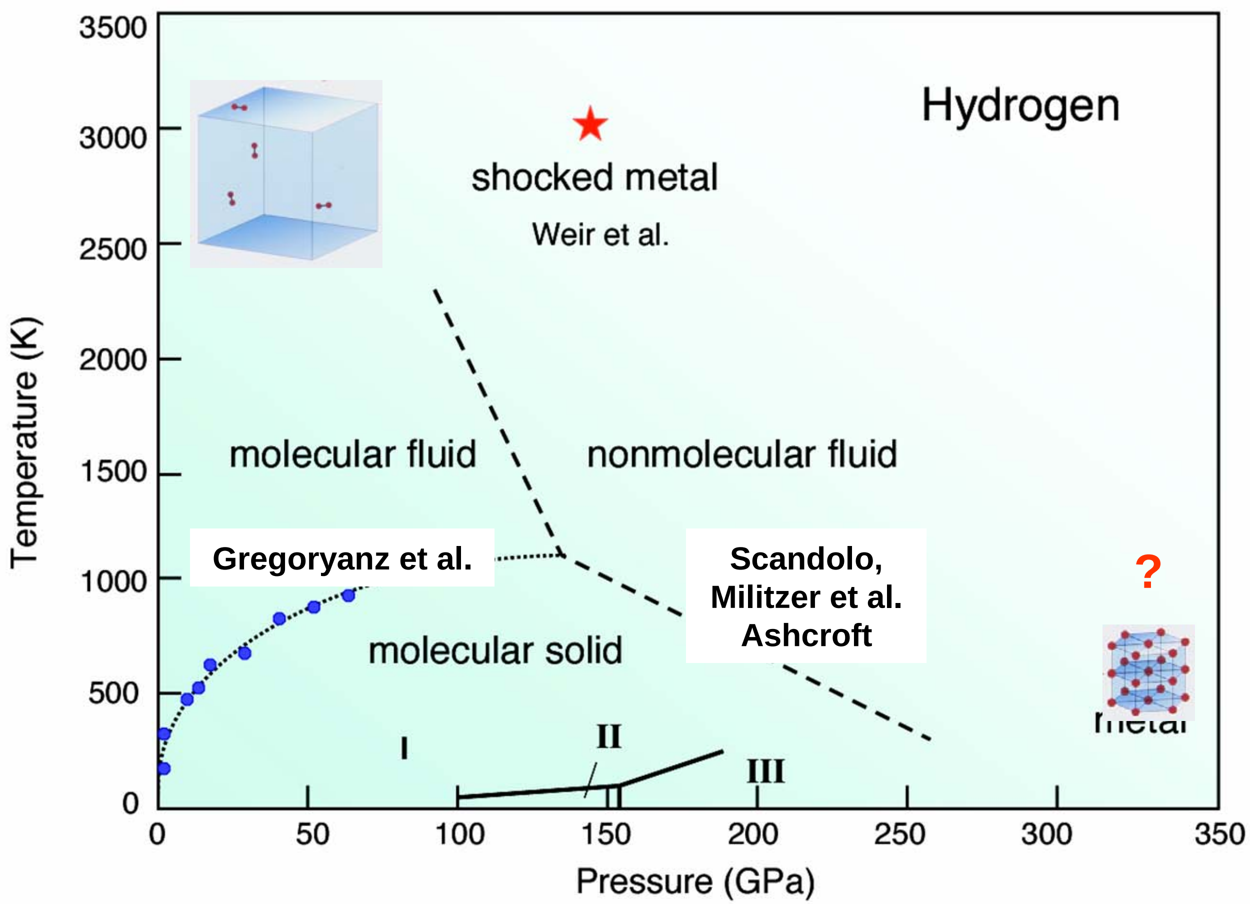


Struzhkin *et al, Nature* (1997)

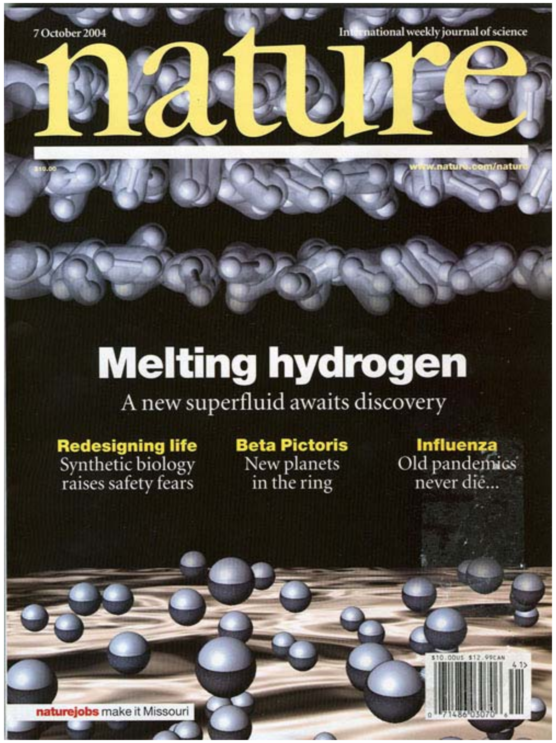


Eremets *et al, Science* (2001)

Hydrogen at Extreme P-T Conditions

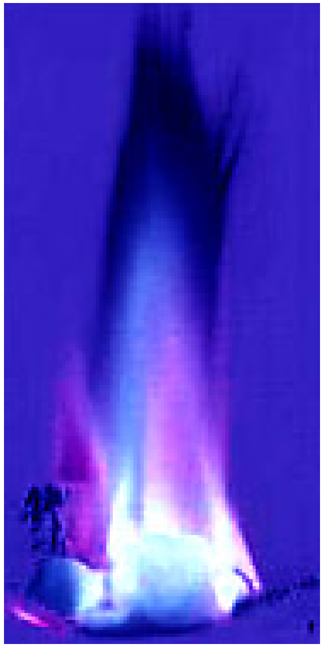


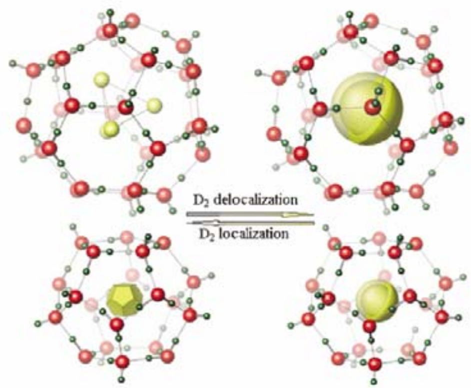
- *TENACITY OF MOLECULAR BOND?*
- *LIQUID GROUND STATE?*
- *HIGH-T_c SUPERCONDUCTOR?*
- *SUPERFLUID?*

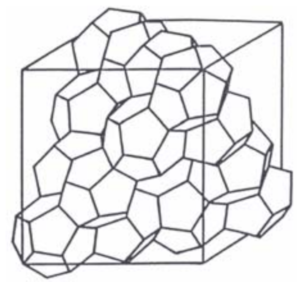


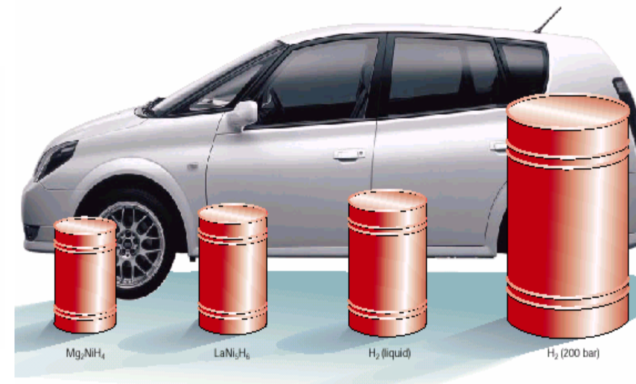
Neil Ashcroft, *PRL* ***92*** (2004)

Pressure creates novel materials -- Examples: hydrogen storage in clathrate



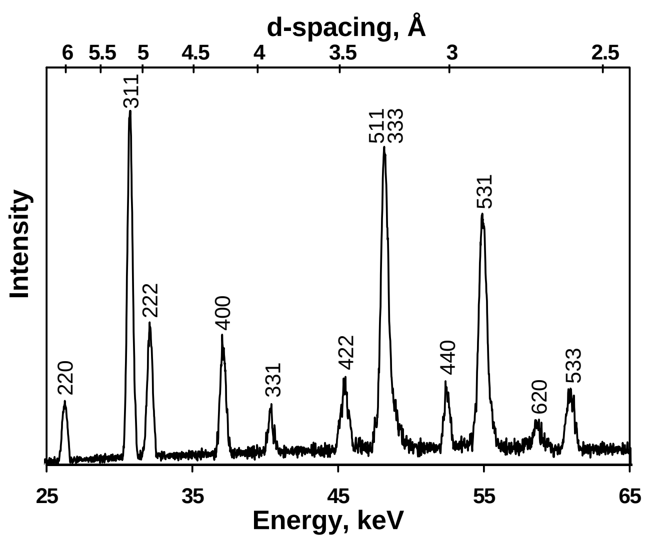


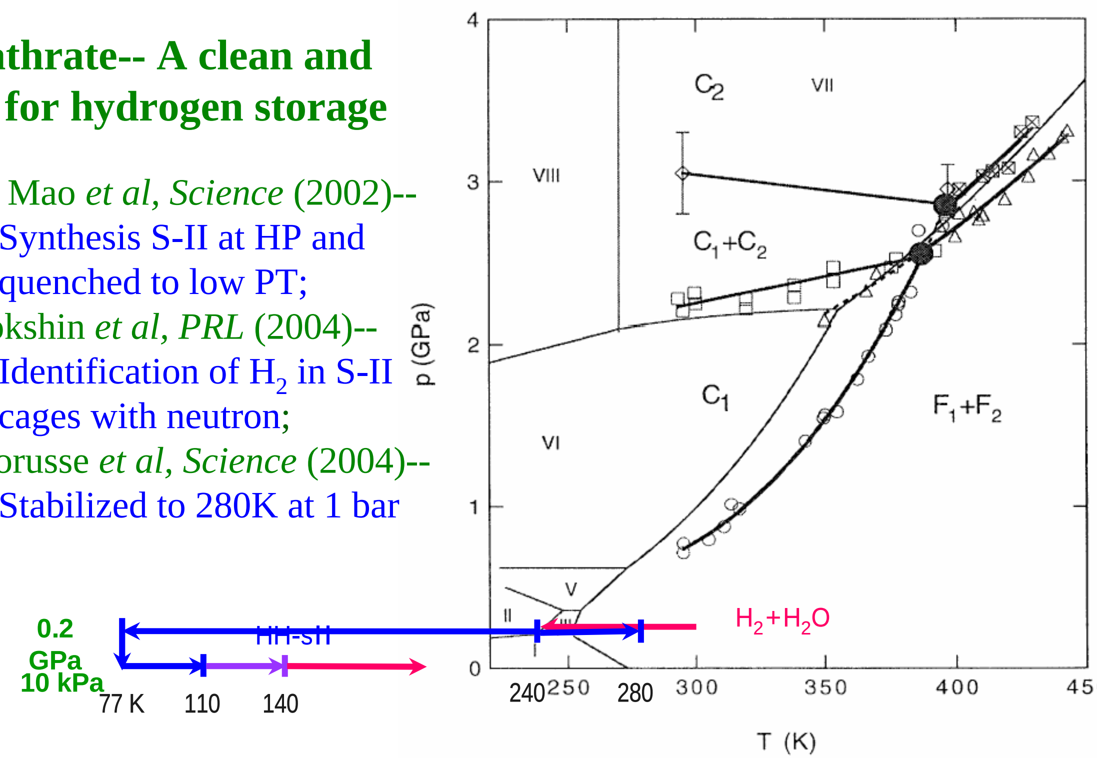




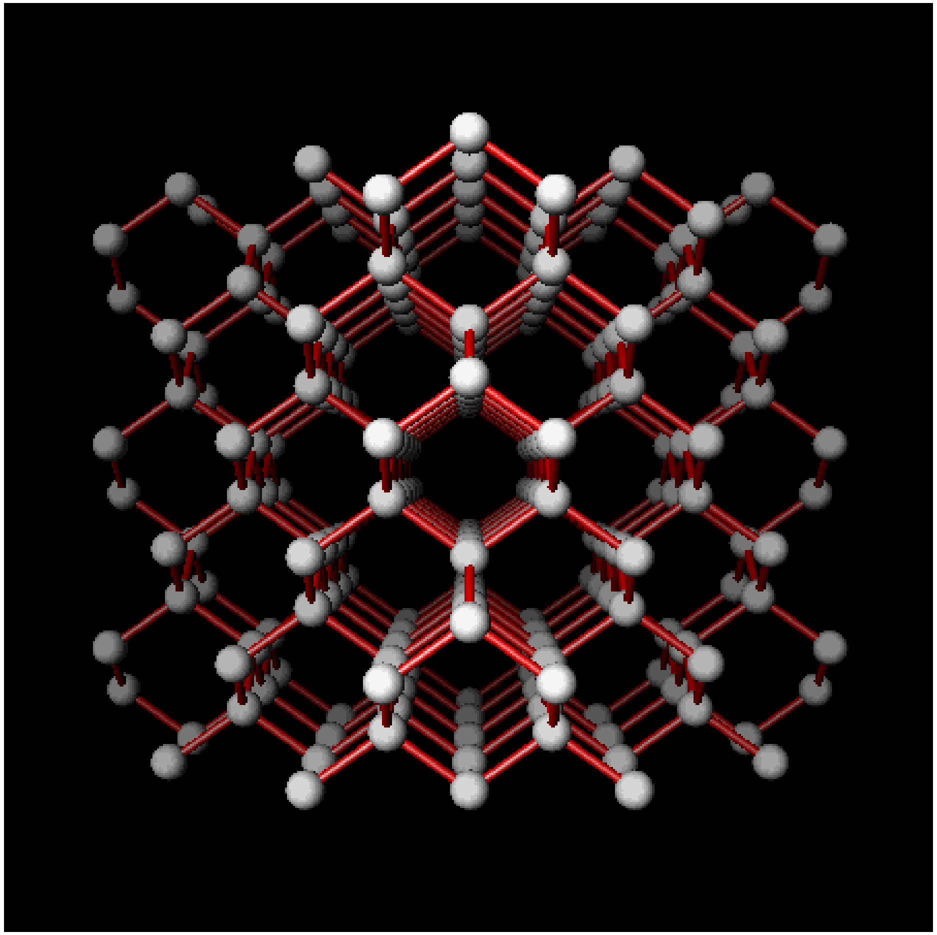
H_2-$2H_2O$ S-II clathrate-- A clean and efficient material for hydrogen storage

W Mao *et al*, *Science* (2002)--
  Synthesis S-II at HP and quenched to low PT;
Lokshin *et al*, *PRL* (2004)--
  Identification of H_2 in S-II cages with neutron;
Florusse *et al*, *Science* (2004)--
  Stabilized to 280K at 1 bar



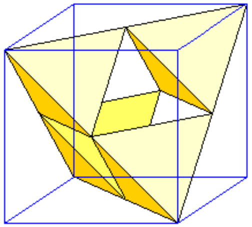


Diamond is a well-known example of a material stable at high *P*, but can be synthesized and used at low P for a wide range of applications.



Unique combination of properties:

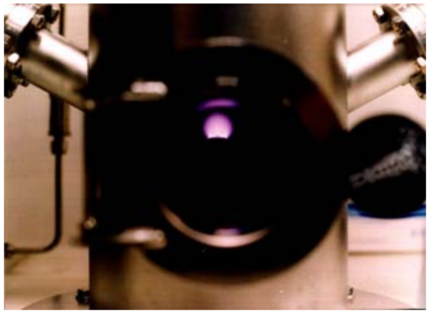
- High hardness
- Low friction
- Low adhesion to other materials
- High thermal conductivity
- Low thermal expansion coefficient
- Wide optical transmission band
- High refractive index
- Chemical inertness
- Biocompatibility
- Radiation hardness
- Electrical insulator
- Excellent electronic properties



Most industrial diamonds are synthesized by high *P-T* process. China is by far the world's largest producer (>85%), but high quality diamonds still depends on import .

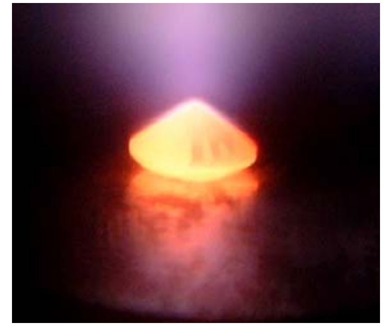
Giant, perfect, single-crystal diamonds can now be grown by chemical vapor deposition (CVD) process at low *P*

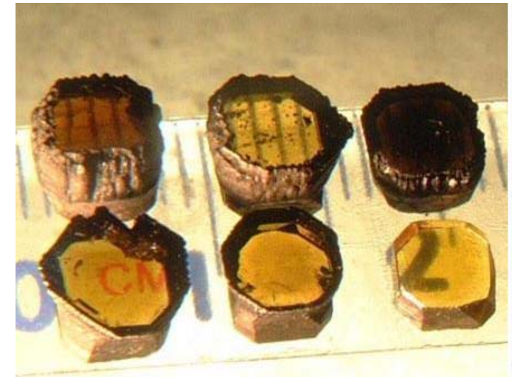
Diamond Growing in a Plasma Reactor

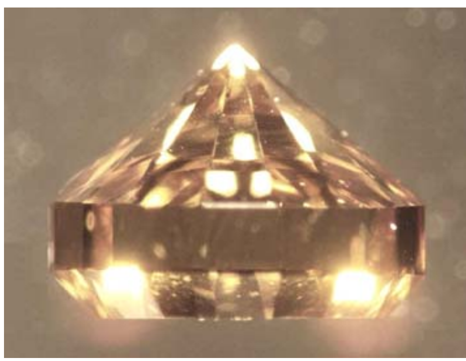


Growth rate improved from 1 μm/hr to 300-500 μm/hr

[Yan *et al*. *PNAS* 99, 12523 (2002)]







Production of regular diamond anvil
- 2.45 mm high
- 0.28 carats
- Grown in 1 day
- reached 200 GPa

W. Mao et al, APL 83, 5190 (2003)
Yan *et al*. *Phys. Stat. Sol.* 201, R27 (2004)

5/16/05 News release:

10 carat, single- crystal, colorless CVD diamond

7 mm diameter, 12 mm length,

Important techniques for high pressure

- Hard x-ray nanoprobe
- Soft coherent scattering and imaging
- High resolution powder diffraction
- Macromolecular crystallography
- Liquid interface
- Inelastic x-ray scattering
- Hard coherent and XPCS/SAXS
- XAFS
- Bio-SAXS
- Photoemission spectroscopy
- ....

How do we make this happen?

Dedicated (BAT) beamlines?

- High Pressure Sciences
  - *X17 at NSLS*
  - *HPCAT at APS*
- Earth Sciences
  - *X1A , X17, X26 at NSLS*
  - *GSECARS at APS*

Infrastructure?

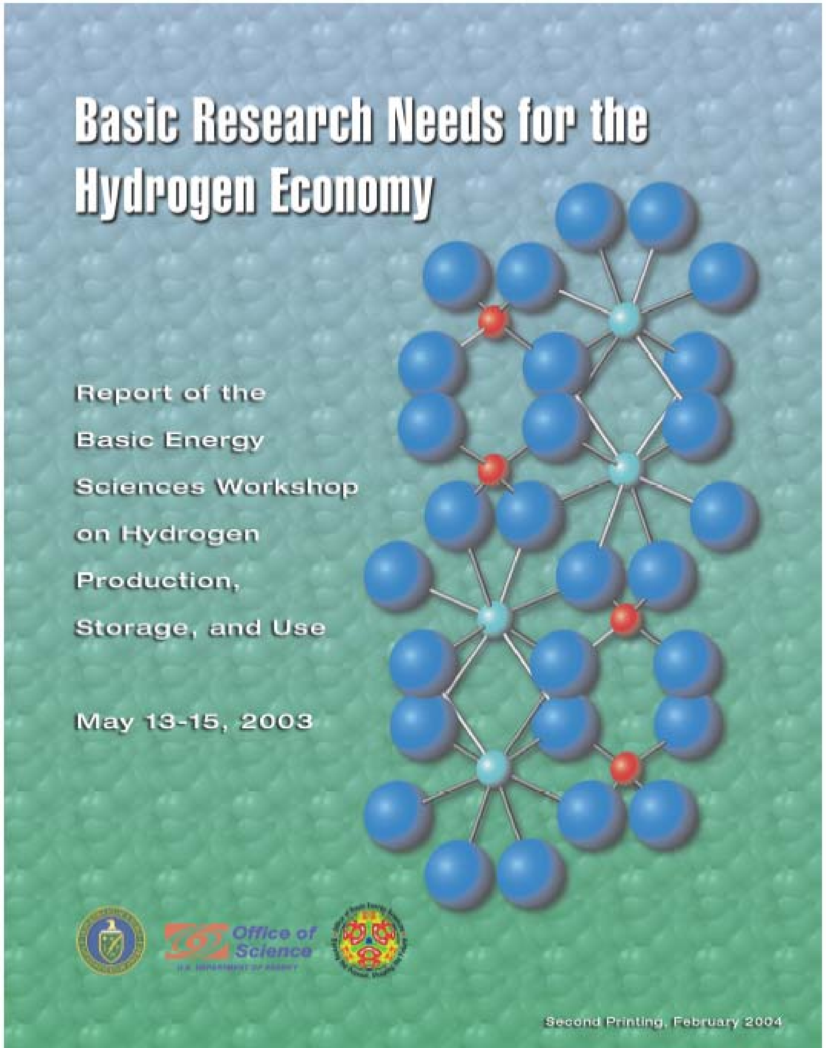
Community drivers, e.g., COMPRES, CDAC

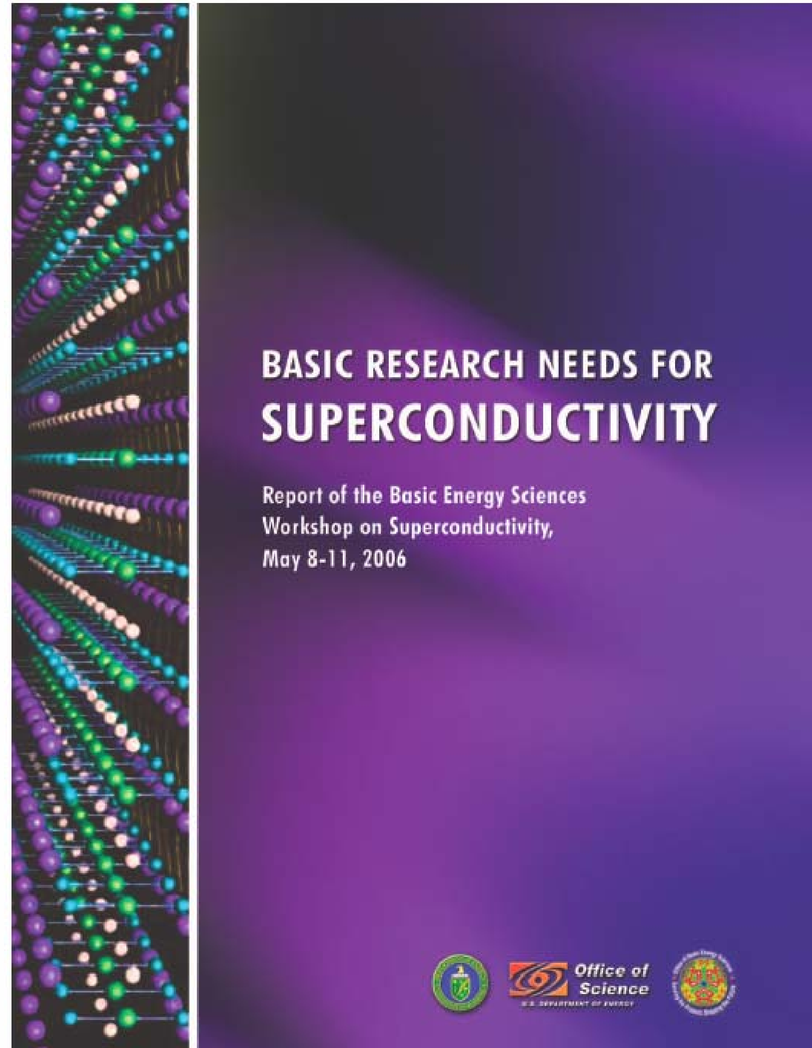
Scientific and technical drivers: HPSynC, JPSI

To access all state-of-the-art NSLS II capabilitiey

Basic Research Needs To Assure A Secure Energy Future

A Report from the
Basic Energy Sciences Advisory Committee


Basic Research Needs for the Hydrogen Economy
Report of the Basic Energy Sciences Workshop on Hydrogen Production, Storage, and Use
May 13-15, 2003
Office of Science
Second Printing, February 2004


BASIC RESEARCH NEEDS FOR SUPERCONDUCTIVITY
Report of the Basic Energy Sciences Workshop on Superconductivity, May 8-11, 2006
Office of Science

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17. Complex Systems: Science for the 21st Century
18. Nanoscale Science, Engineering and Technology Research Directions

Conclusions for High Pressure Sciences at NSLSII

- Sciencific frontiers
  Multidisciplinary physical sciences

- Techniques
  All NSLS-II beamlines
  General HP BAT beamline

- Key enablers
  DOE support, HPSynC, JPSI