High Pressure Hydrogen: CW Structures and Pulsed Temperatures

Isaac F. Silvera
Lyman Laboratory of Physics
Harvard University

The Hydrogens at High Pressure

Hydrogens: Hydrogen and its isotopes

D2, HD

	mass	nuclear spin	
Hydrogen	2	1/2	fermion
Deuterium	4	1	boson
Hydrogen Deuteride	3	3/2	Maxwell
~~Tritium~~ radioactive	6	1/2	fermion-

The Hydrogens at High Pressure

Hydrogens: Hydrogen and its isotopes

D2, HD

Unanswered Questions:

High pressure structural phases

Molecular or atomic

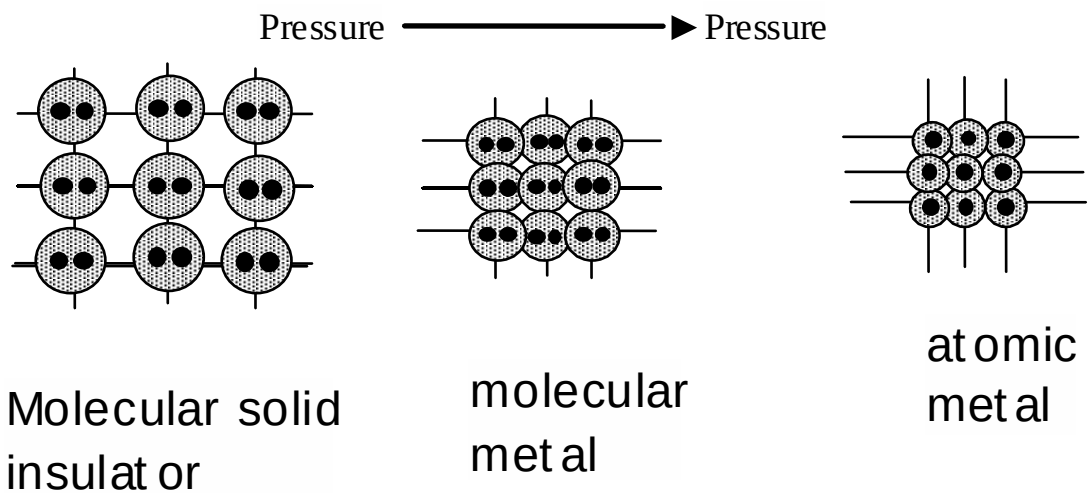
Insulating or metallic

Liquid at high pressure and T=0 K

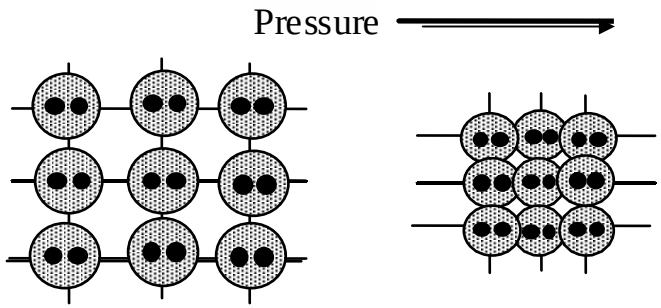
Superconducting or normal metal

Superfluidity

The Wigner-Huntington Transition to Atomic Metallic Hydrogen (1935)



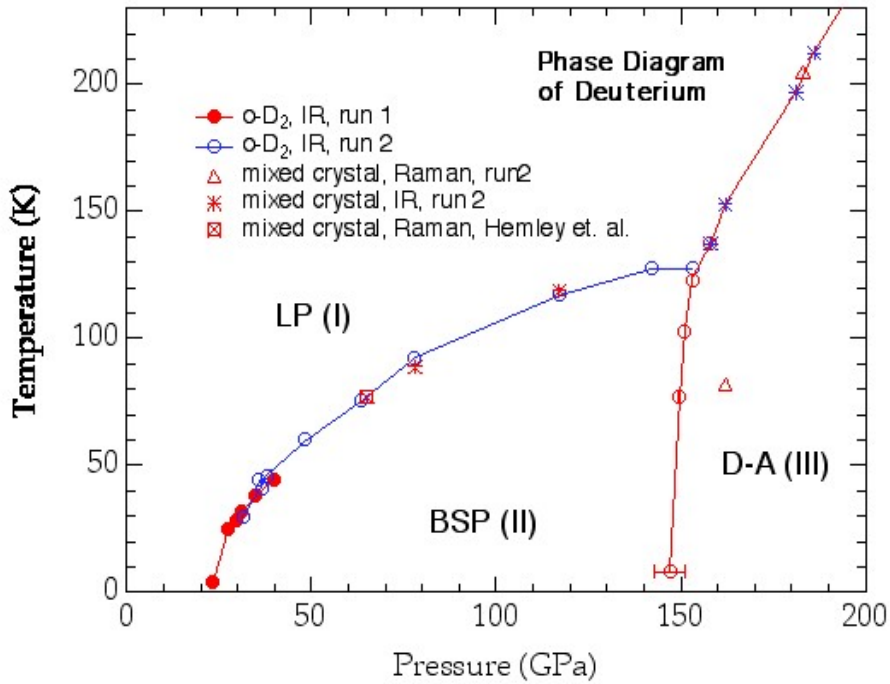
The Known High Pressure Molecular Insulating Phases



Molecular solid insulator

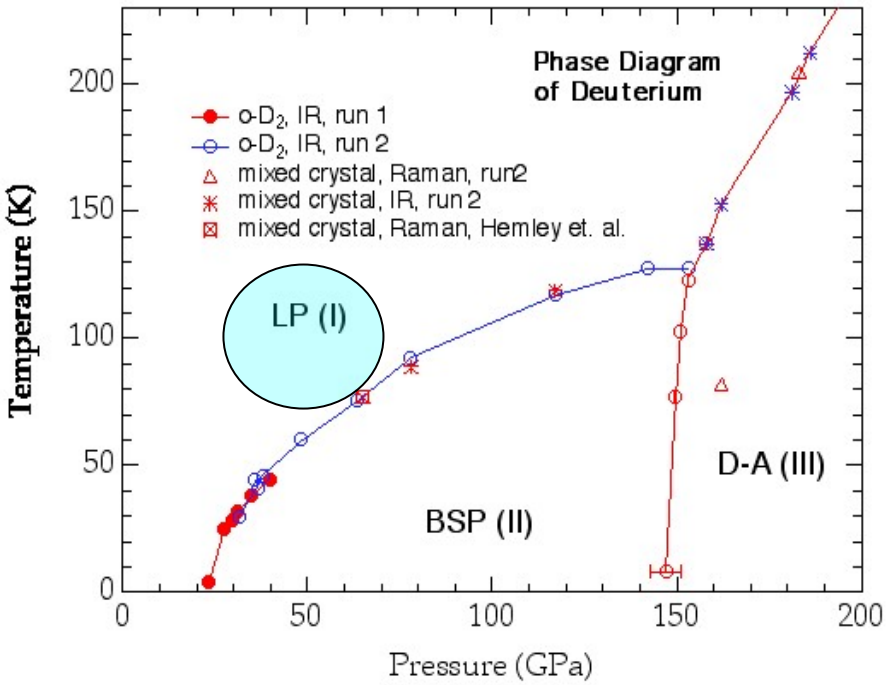
molecular

The Experimentally Visited High Pressure Phases

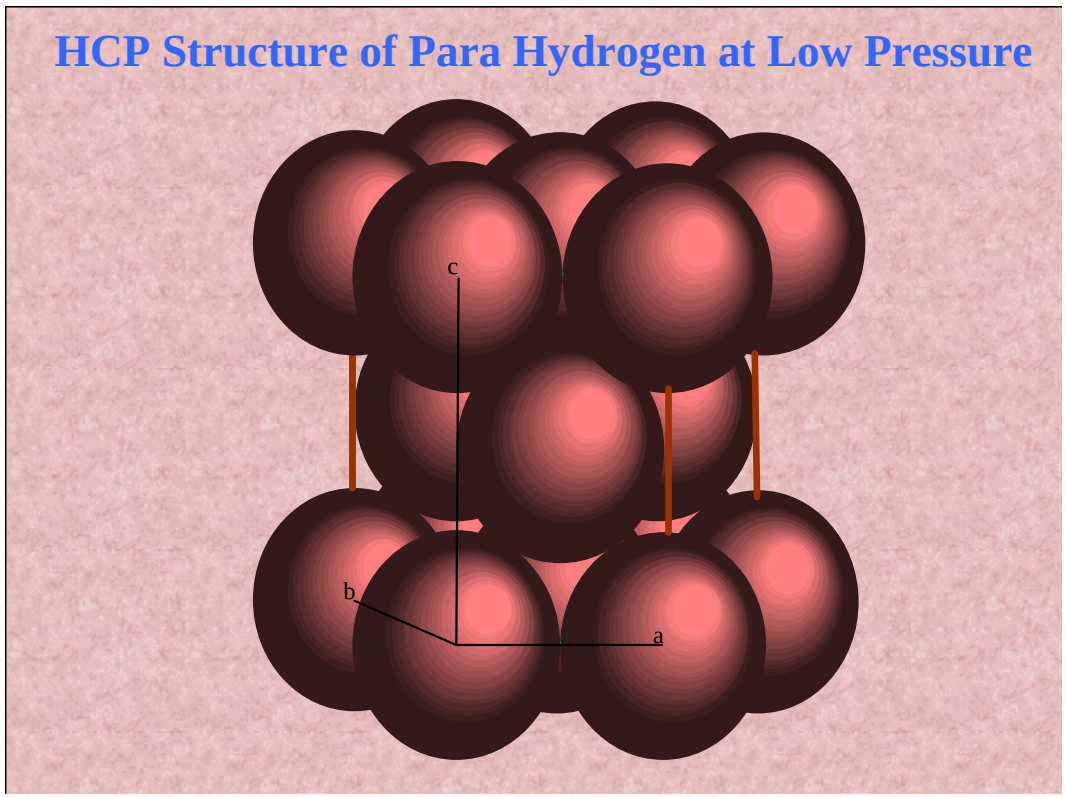


The LP (low pressure) phase in Ortho Deuterium (J=0)

(Hydrogen is similar)



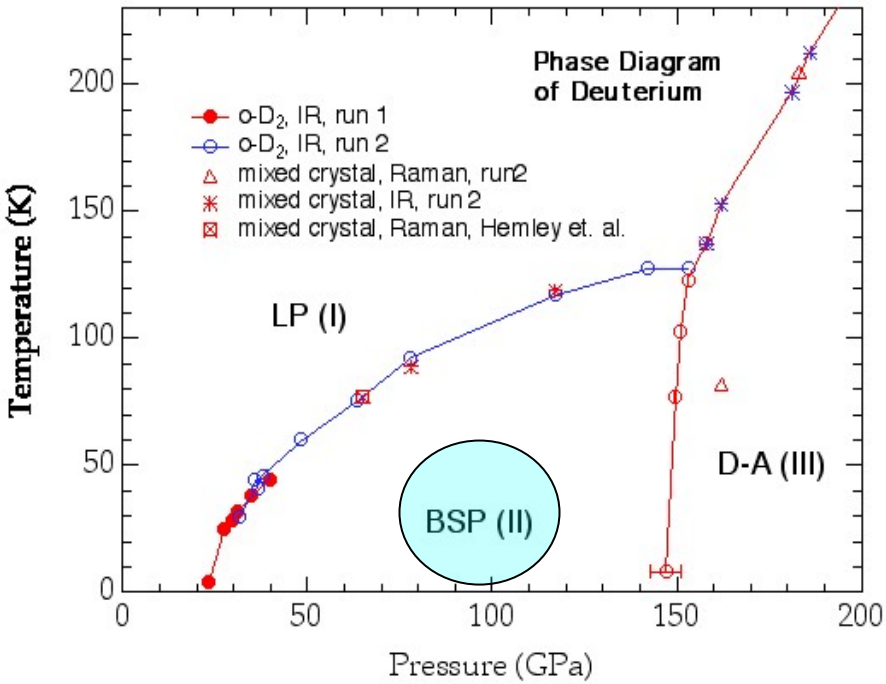
Zero pressure: Both para hydrogen and ortho hydrogen crystallize in an HCP lattice. Para remains HCP to P=0;



Para molecules have spherical quantum mechanical distributions;

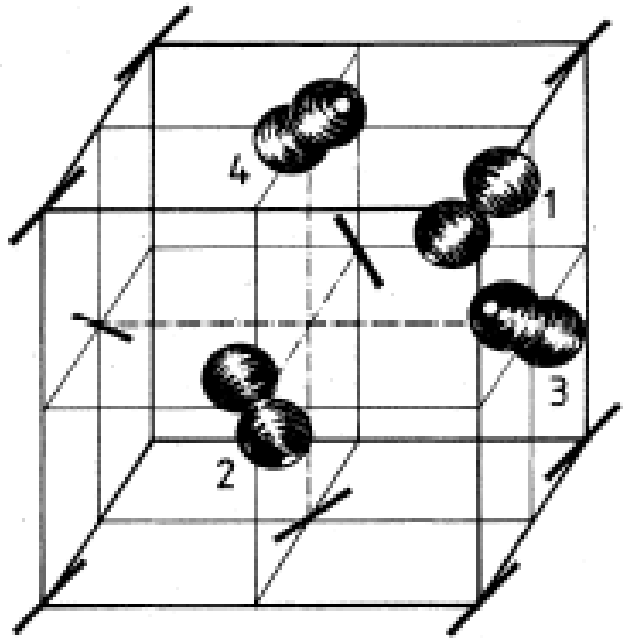
They are not orientationally disordered, but in a "symmetric many-body state"

The BSP in Ortho Deuterium (J=0) (Hydrogen is similar)



The BSP phase is of orientational order. Originally predicted to be Pa3, but recently identified as P3-bar (in deuterium) by Goncharenko and Loubeyre (neutron scattering)

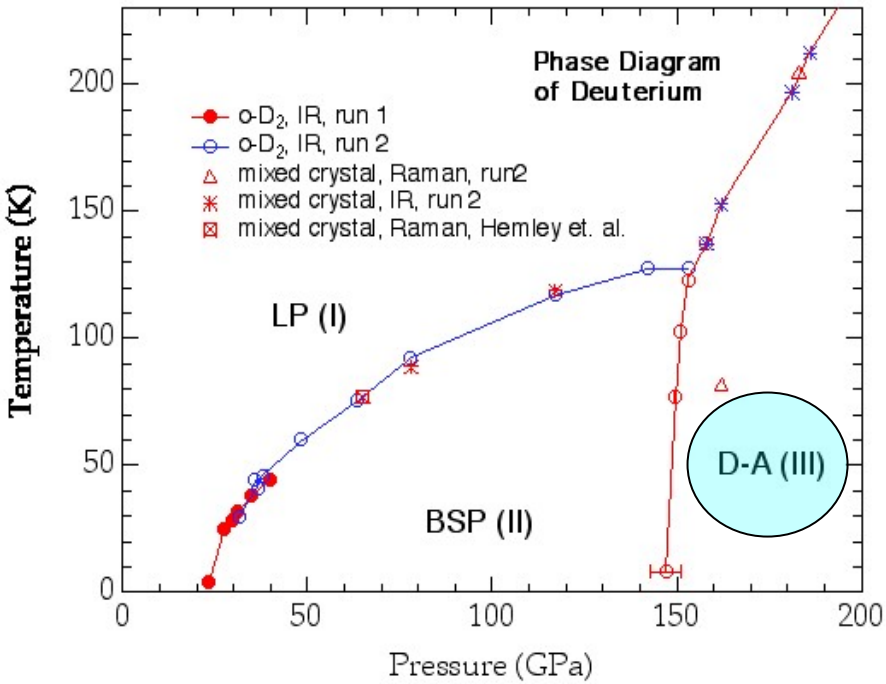
Pa3 structure from Raman Scattering spectra of librons at zero pressure.



P3-bar is similar but more complicated-not on fcc but hexagonal underlying structure of molecular centers.

Above T_C the molecules are orientationally disordered.

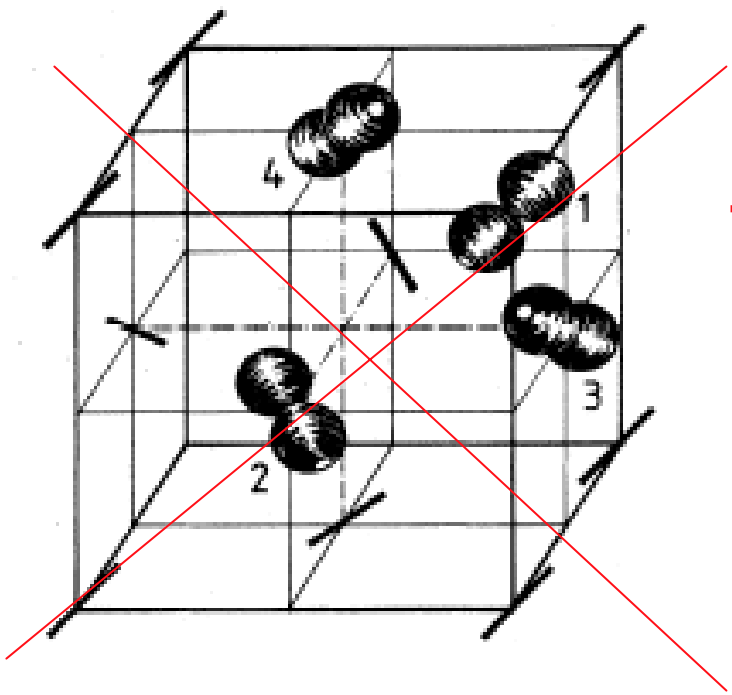
The A-phase in Ortho Deuterium (J=0) (Hydrogen and HD are similar)



The A-phases: molecules are orientationally ordered but not in well defined spherical harmonic quantum states.

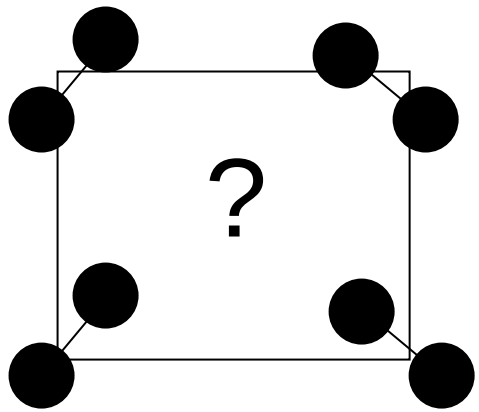
Molecules are in classical ball and stick states.

The solid is an insulator, not a metal!

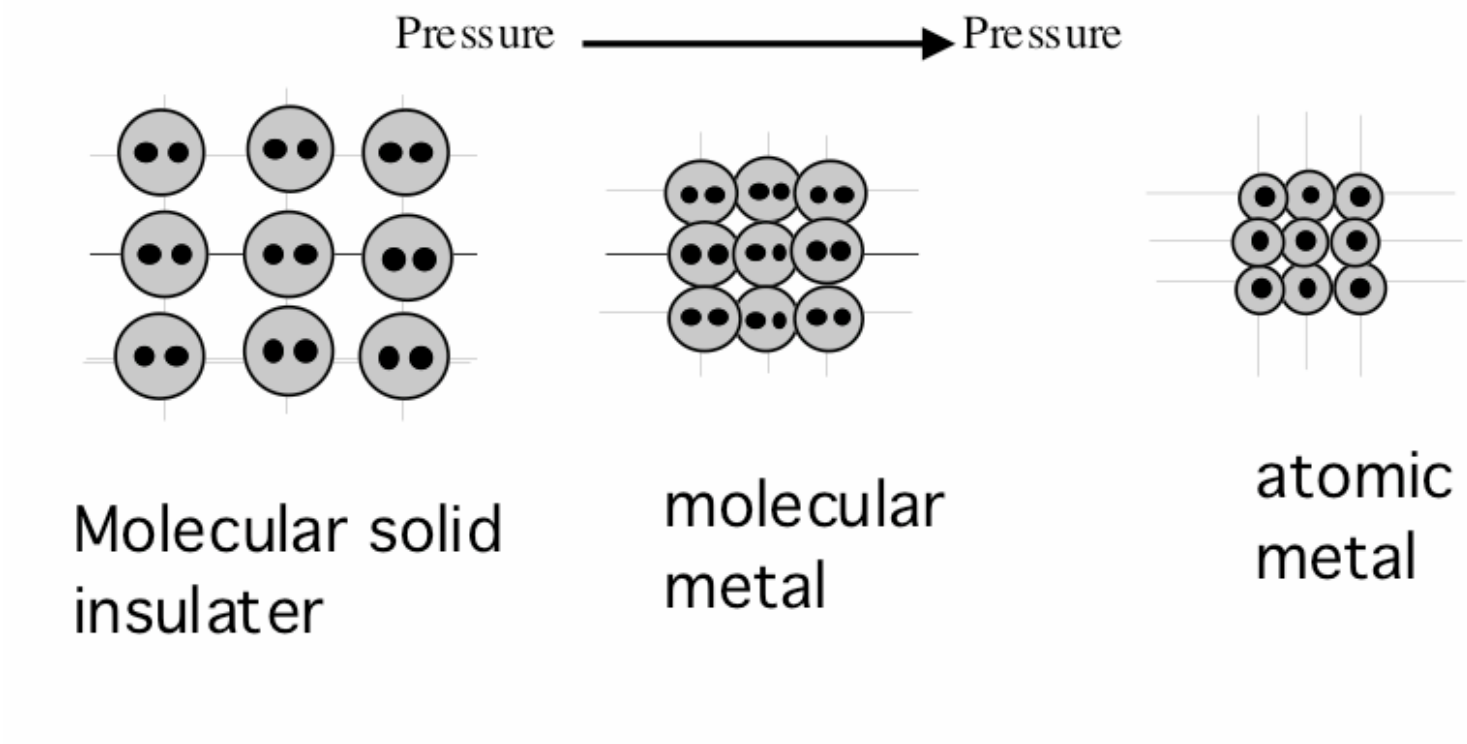


The structure

is not known



Solid Metallic Hydrogen



Solid Metallic Hydrogen: Theory, Predictions

- **Metal Insulator Transition in Solid Hydrogen--0.25 megabar**
  Wigner, Huntington, 1935
- **High Temperature Superconductivity in Atomic Metallic Hydrogen**
  Ashcroft , 1968
- **Molecular metal at high pressure**
  Harris, Monkhorst, 1971
- **Metastability, liquid at T=0 K**
  Brovman, Kagan, Kholas, 1972-- Salpeter-perhaps unstable to recombination
- **Calculations of the critical pressure for metallization-- 1 to 20 megabar**
  A few dozen published and unpublished calculations by a large number of researchers
  1950's to present day-- Difficulty with ZPM, fermion node problem, assumed structures
- **Negative slope in the melting curve; new phase lines in the melt; possible liquid at T=0 K**
  Scandolo, 2003; Bonev et al, 2004; Ashcroft et al-- quantum-classical MD calculation
- **Two component Superconductivity &Superfluidity in high-pressure liquid hydrogen**
  Babaev, Sudbe, Ashcroft-- electron-proton coupling challenge

Highest pressures in solid hydrogen in a DAC ~350 GPa--not yet metallic

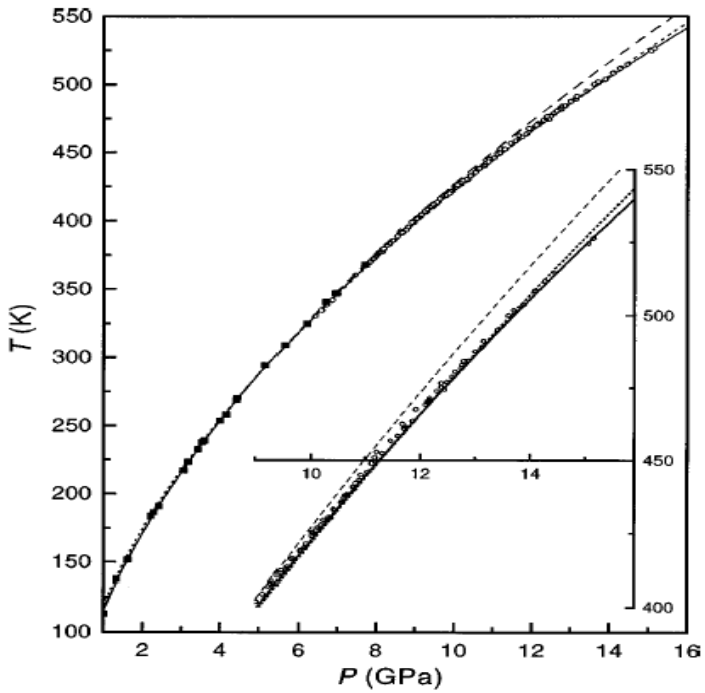
Sample sizes-diameters- in a DAC

~10-30 microns

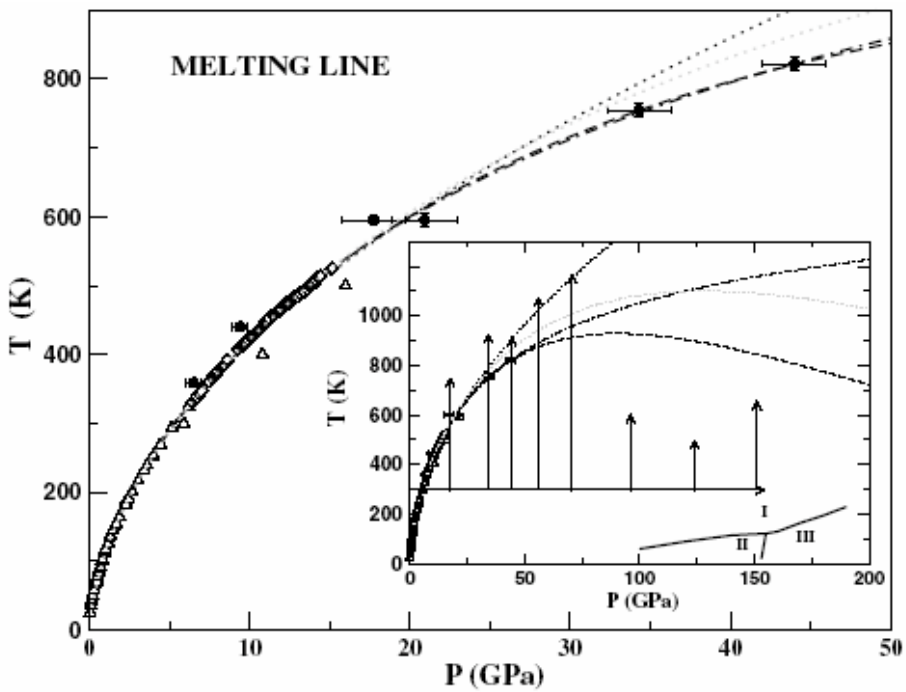
The melting line of hydrogen and the states at very high pressures

Melting Line of Hydrogen Measurements

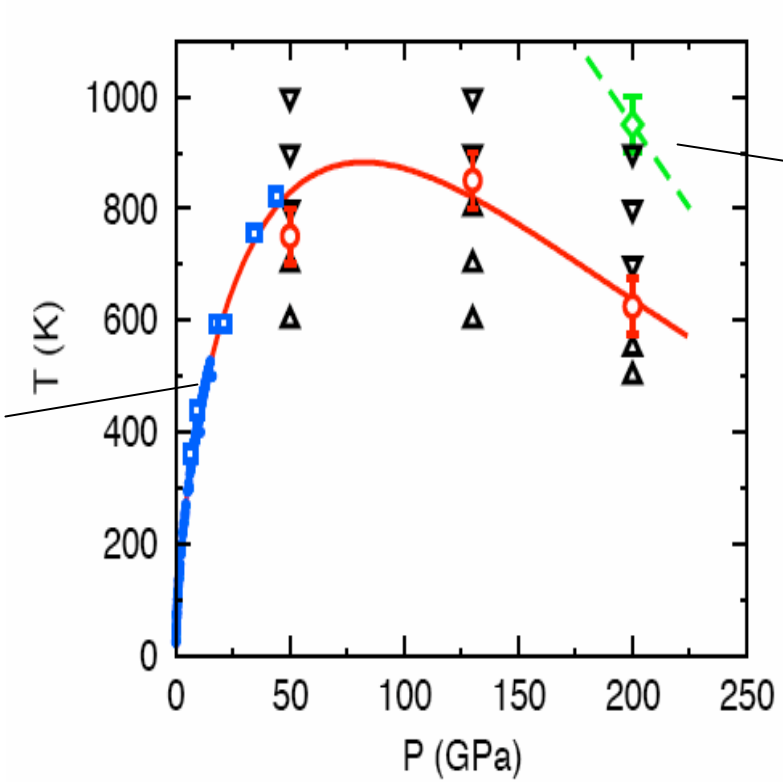
Ohmic Heating in a DAC
Datchi, Loubeyre,LeToullec
PRB 61.6535 (2000)



Ohmic heating in a DAC
Raman detection of melting
Gregoryanz, Goncharov, Matsuishi, Mao, Hemley, Phys. Rev. Lett. 90, 175701-4 (2003).



Melting line prediction from Molecular Dynamics Calculation



The predicted high pressure melt line of hydrogen. Above the dashed line molecules are predicted to dissociate.

S. A. Bonev, E. Schwegler, T. Ogitsu, and G. Galli, Nature 431, 669 (2004).

Will high pressure hydrogen be an atomic metallic liquid at T=0 K?

Babaev,Sudbe, &Ashcroft predict possible

- Superconducting electrons
- Superconducting protons
- Superfluid properties.

Possible limitations for study of the high temperature melting line.

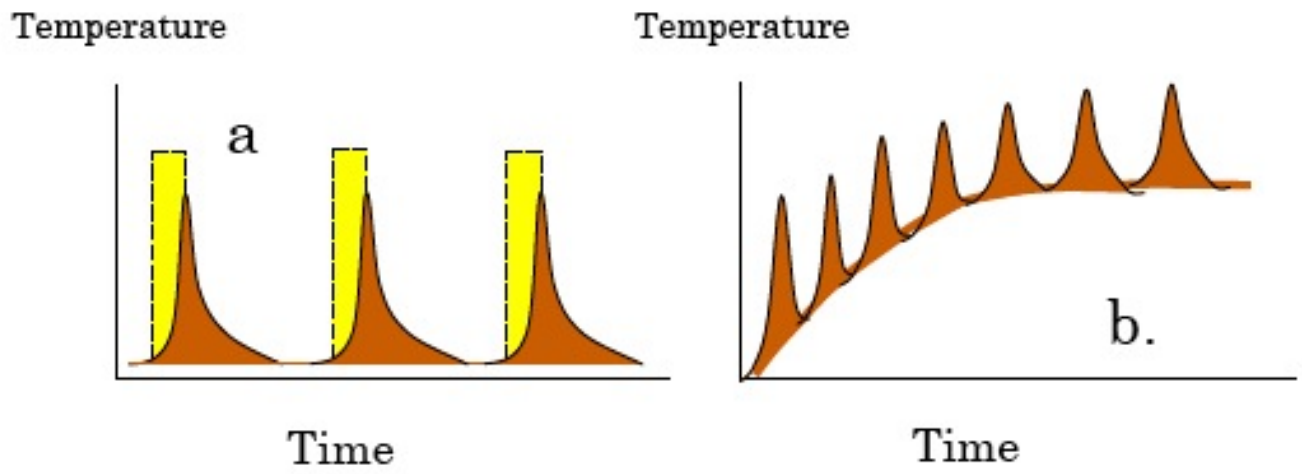
At high temperatures hydrogen diffuses into the diamonds which embrittle and fail.

Solution: pulsed laser heating.

Pulsed laser heating

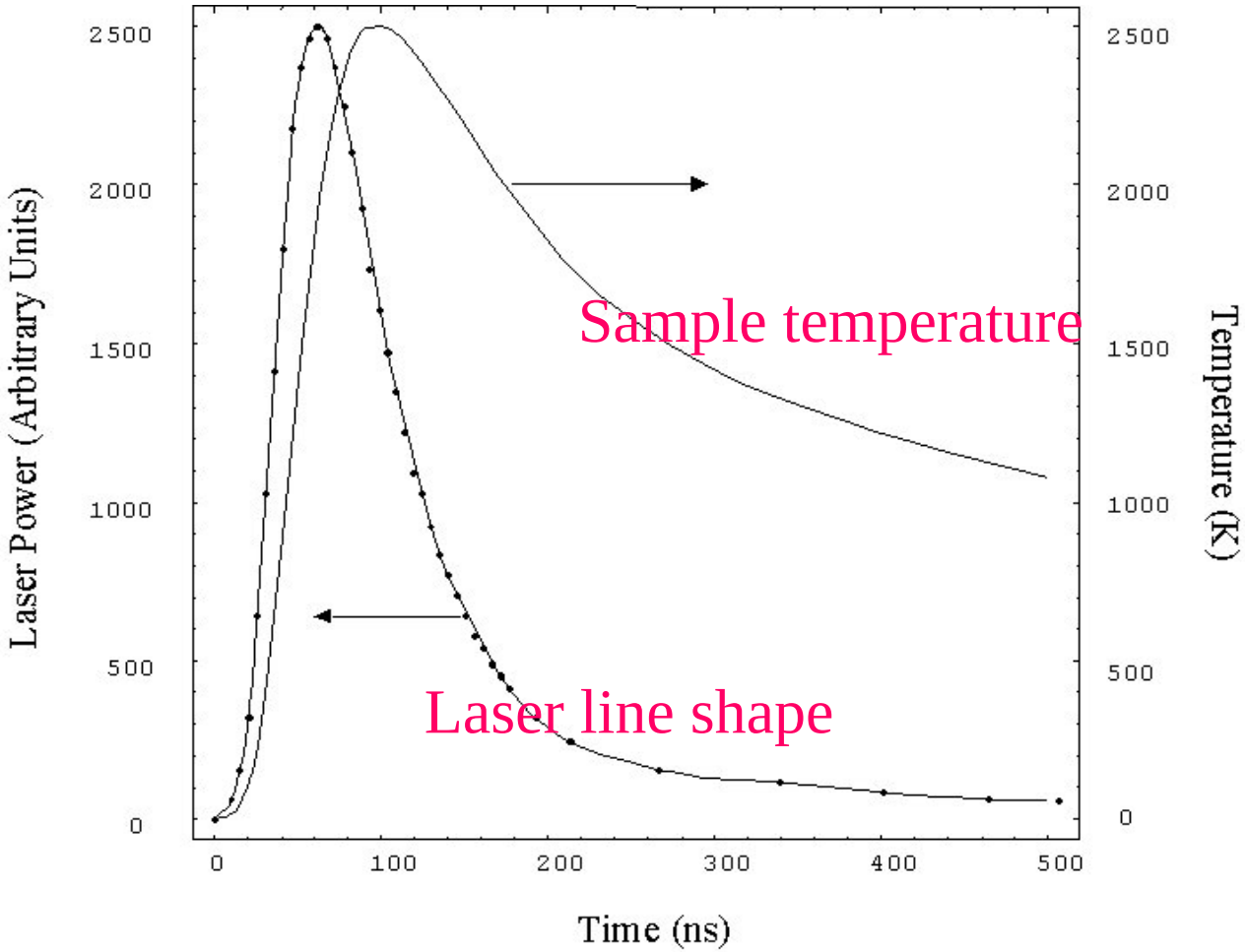
Sufficient time to heat to local equilibrium;

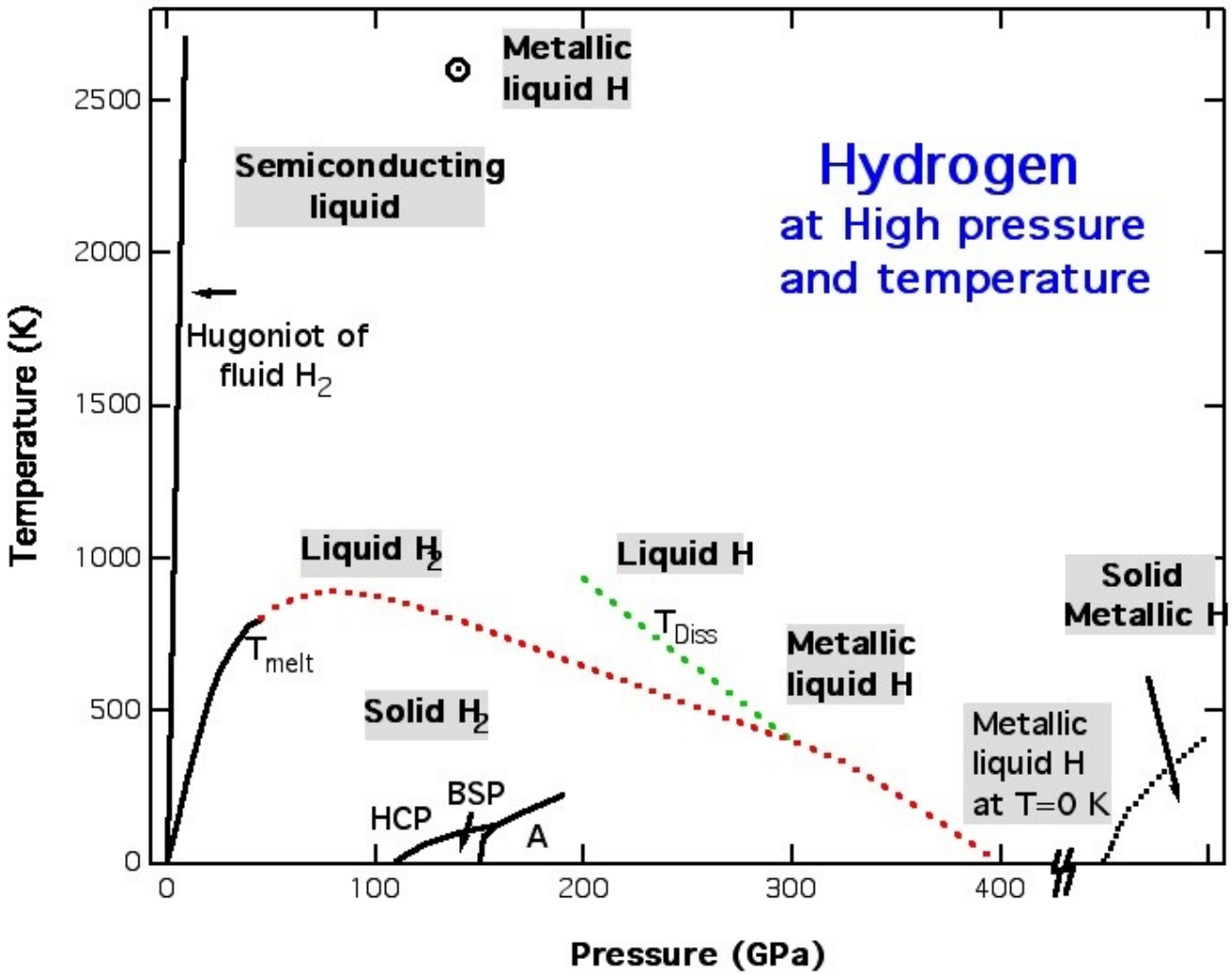
Insufficient time for diffusion.



Pulsed laser heating:

Laser Power Line Shape and Sample Temperature Line Shape




Metallic
liquid H
Semiconducting
liquid
Hydrogen
at High pressure
and temperature
Hugoniot of
fluid H_2
Liquid H_2
Liquid H
T_{Diss}
T_{melt}
Metallic
liquid H
Solid
Metallic H
Solid H_2
Metallic
liquid H
at T=0 K
BSP
HCP
A
Temperature (K)
Pressure (GPa)
0
500
1000
1500
2000
2500
0
100
200
300
400

Challenges to be met by the new ERL x-ray source:

Assuming samples pressurized in DACs and sample sizes very small

Static Measurements

- Structure of BSP for H2, HD
- Structure of the A-phases
- Structure of metallic hydrogen

Dynamic measurements

Synchronize x-ray pulse to laser heating pulse:

Determine high Pressure-high Temperature

- Structural Phases
- Melting
- Molecular-atomic dissociation line
- Metallic? Superfluid?

xx

xx