

Core Mineral Physics



Guillaume MORARD



Plan of the lesson

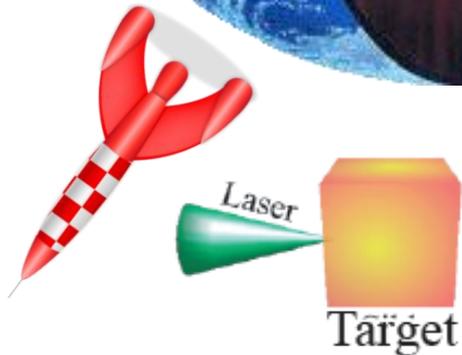
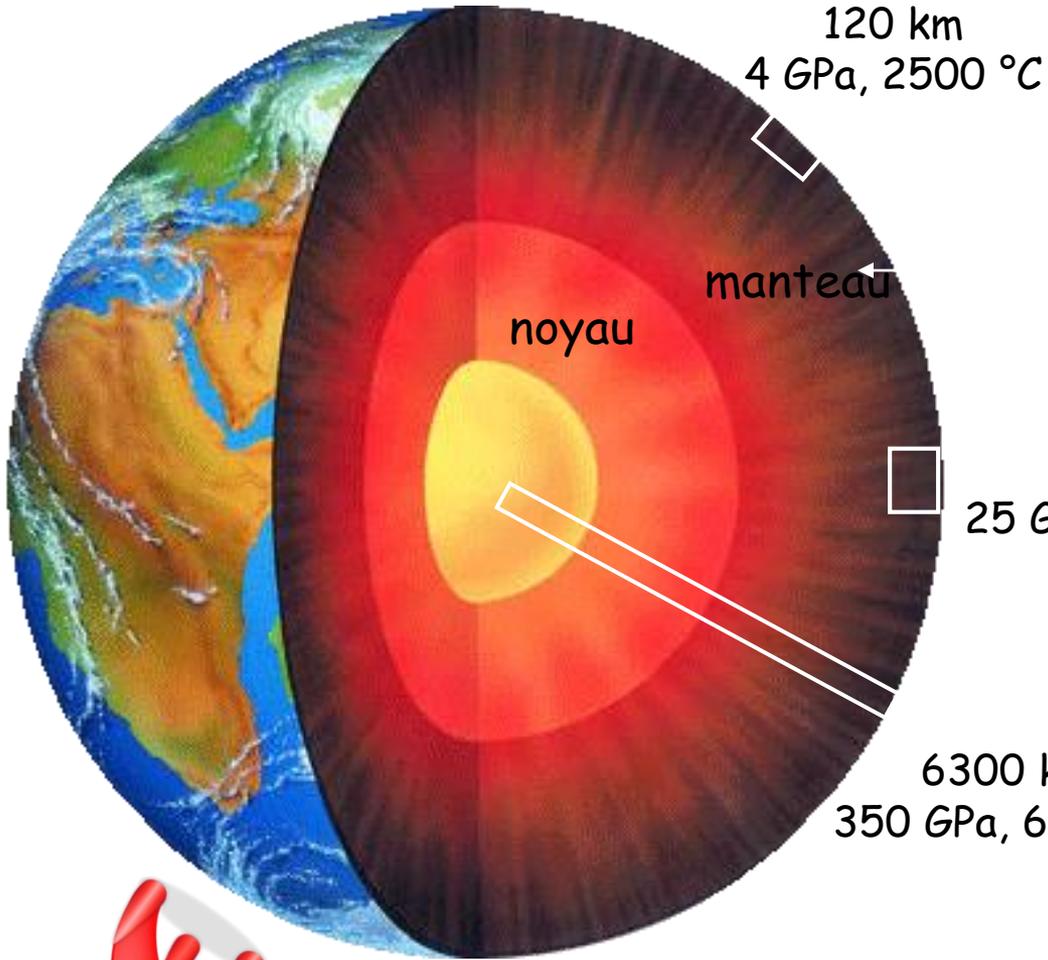
-Compressing stuff



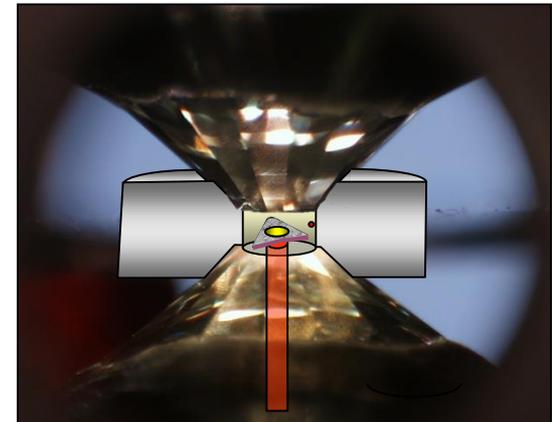
-Then think ...



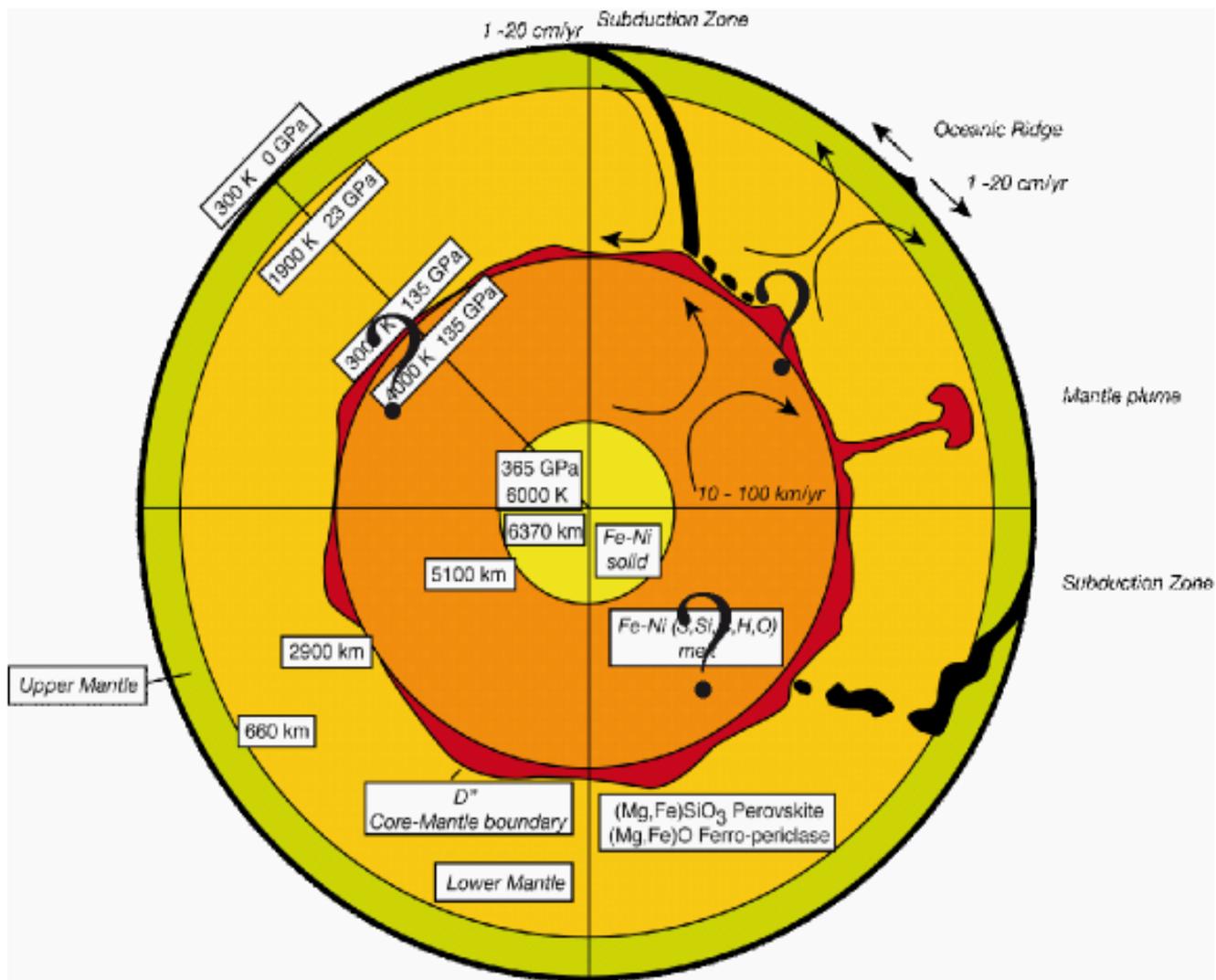
Experiments HP-HT

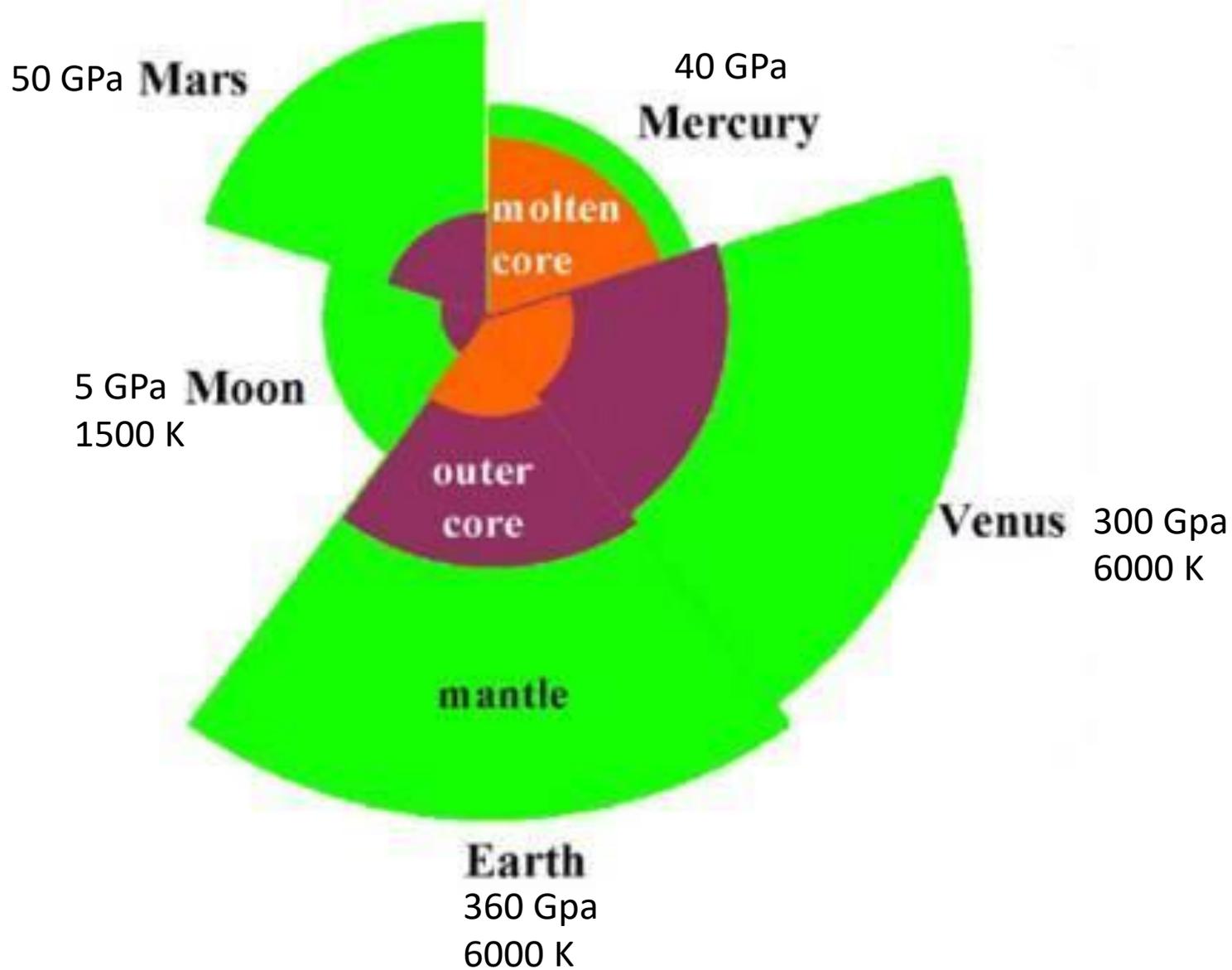


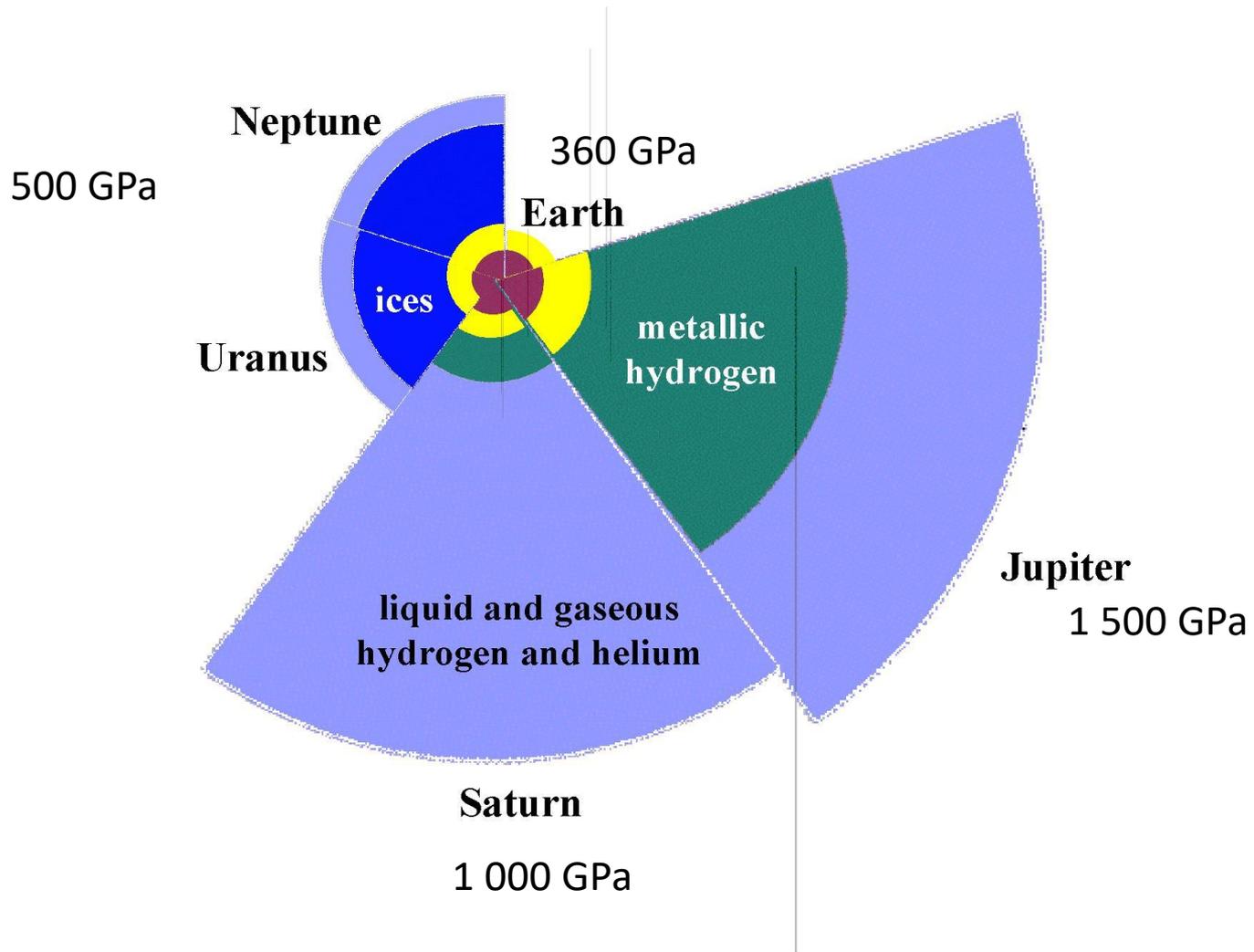
Intérieur des exoplanètes
1 TPa, $T > 10\,000\text{ °C}$
Mais sur 1-2 ns



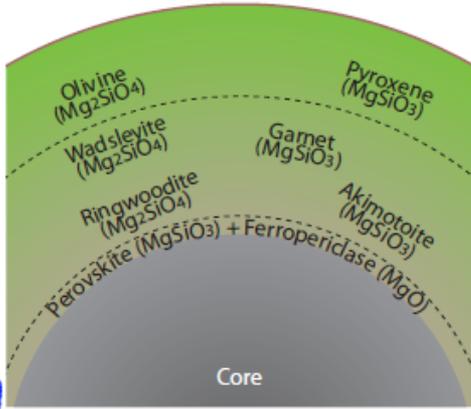
Internal structure of the Earth



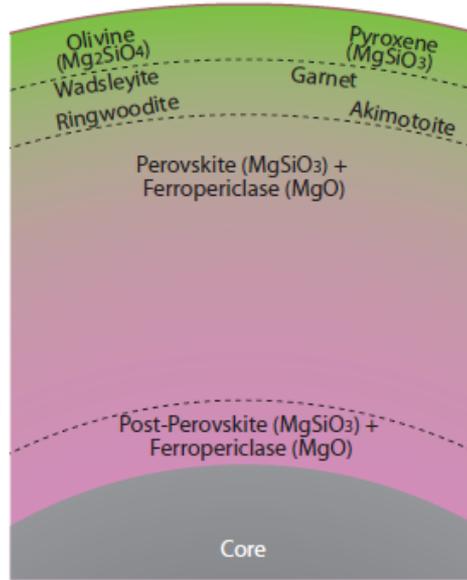




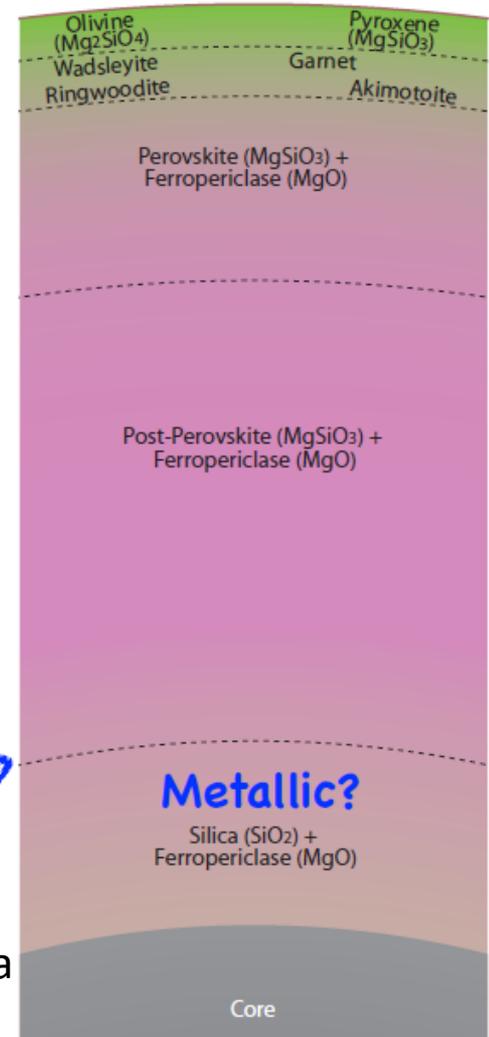
Mars



Earth



Super-Earth



~20 GPa

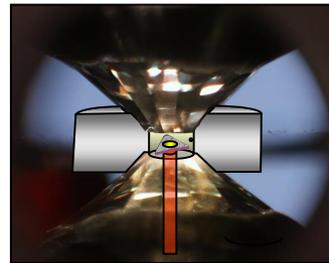
136 GPa

~1000 GPa

CHOCs !!!

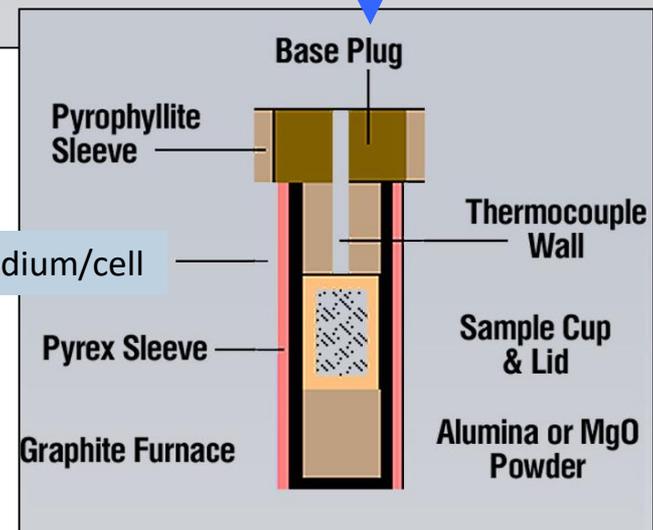
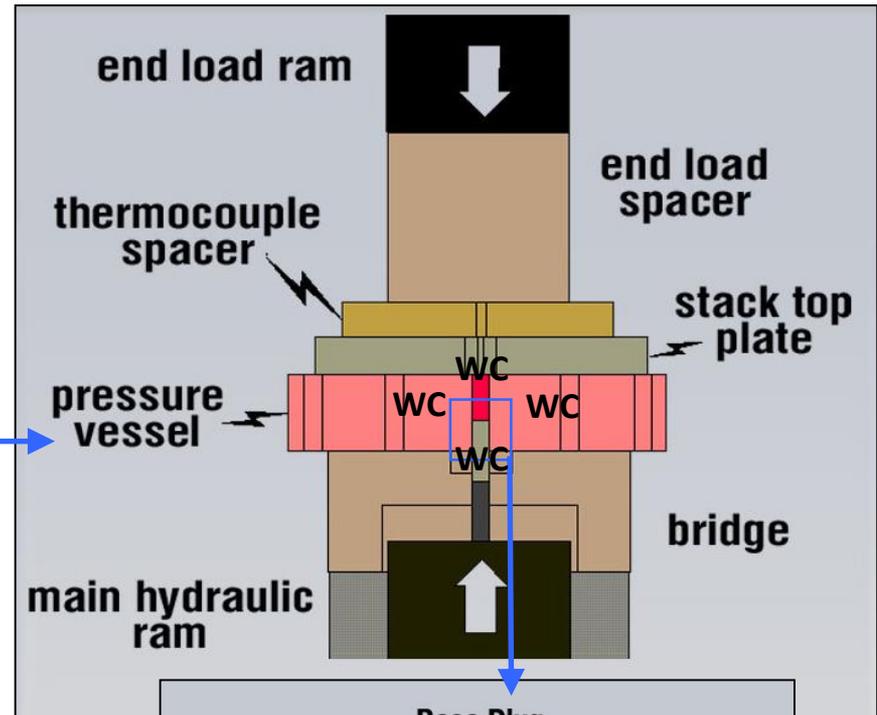


Presse multi-enclumes



Cellule à enclumes de diamants

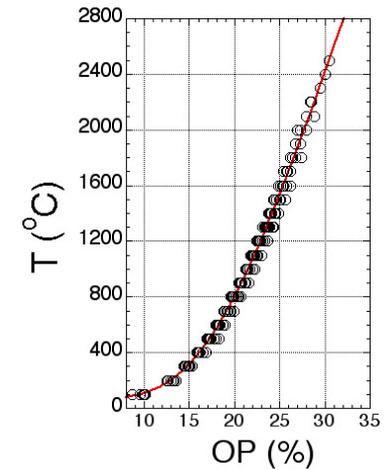
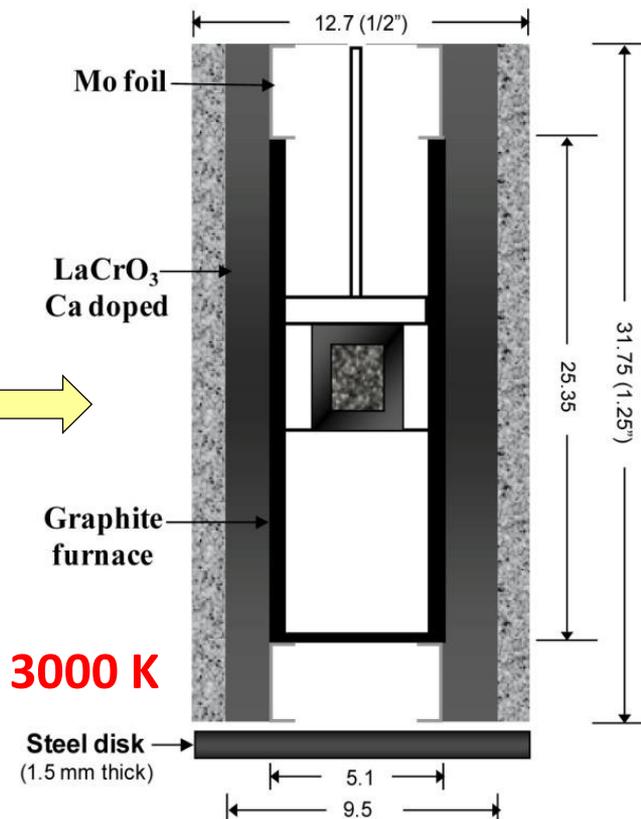
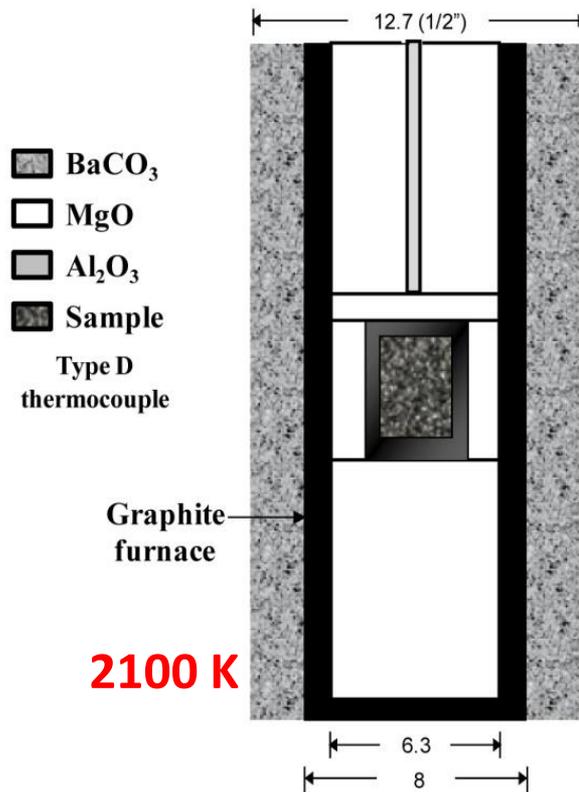
Hydraulic press - Piston cylinder



Pressure is directly derived from
The size of the piston \varnothing
BUT friction loss

Hydraulic press - Piston cylinder

High T assemblies



Resistive furnace

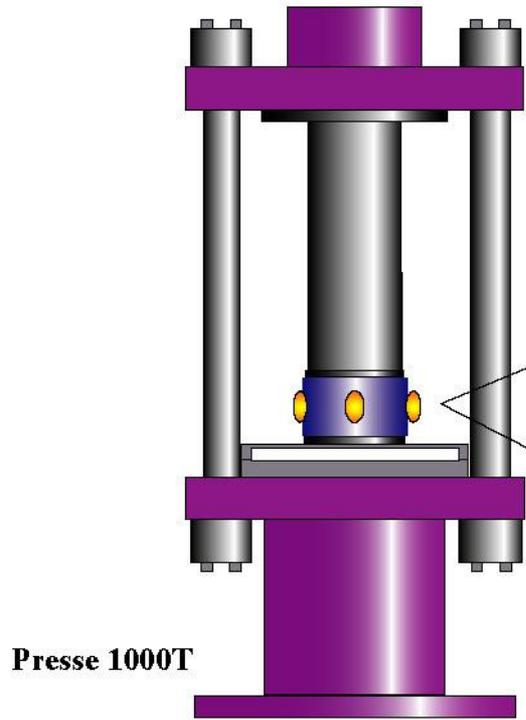
Temperature measured using thermocouple

Hydraulic press – Multi-anvil press

Working range

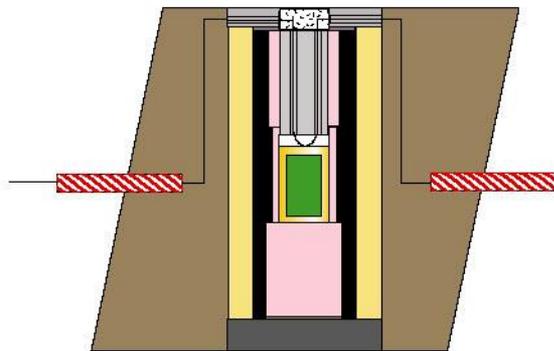
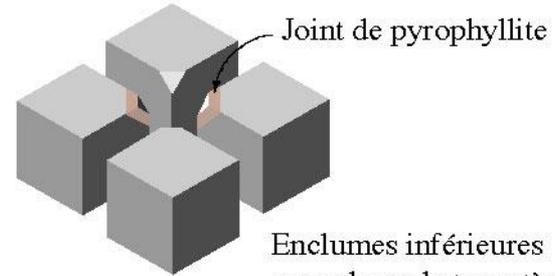
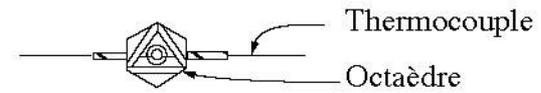
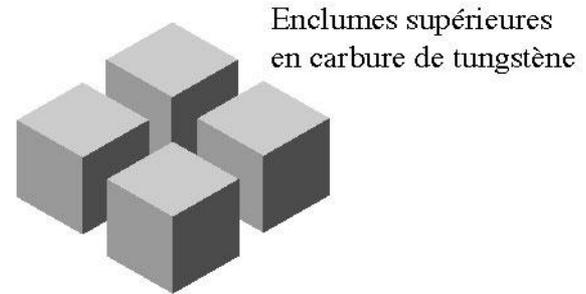
- Pressure : 3 - 26 GPa (carbides); 80-100 GPa (sintered diamonds)
- Temperature : RT to 2500°C
- Duration : several days at $T < 1600^{\circ}\text{C}$

PRESSE MULTIENCLUMES



Presse 1000T

Assemblage cubique

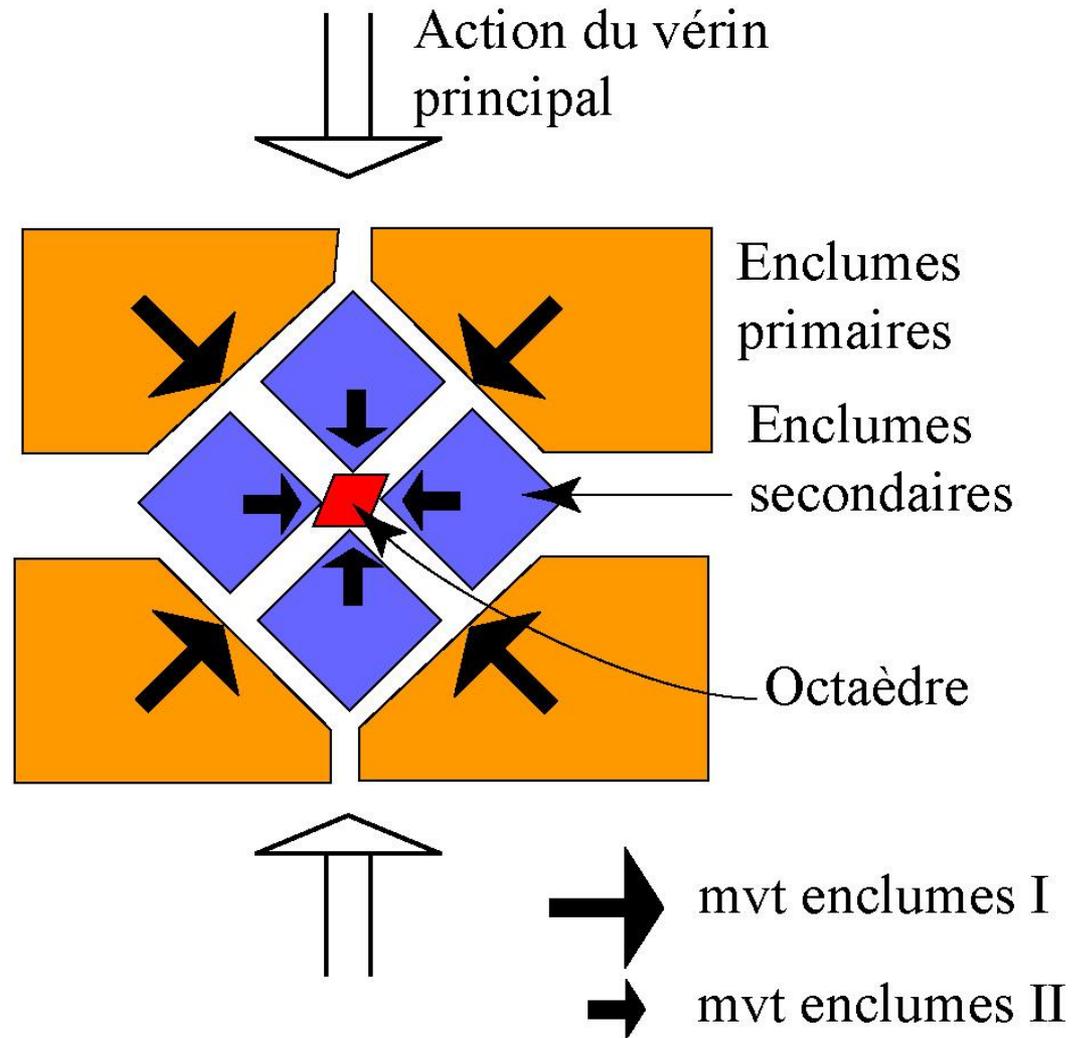
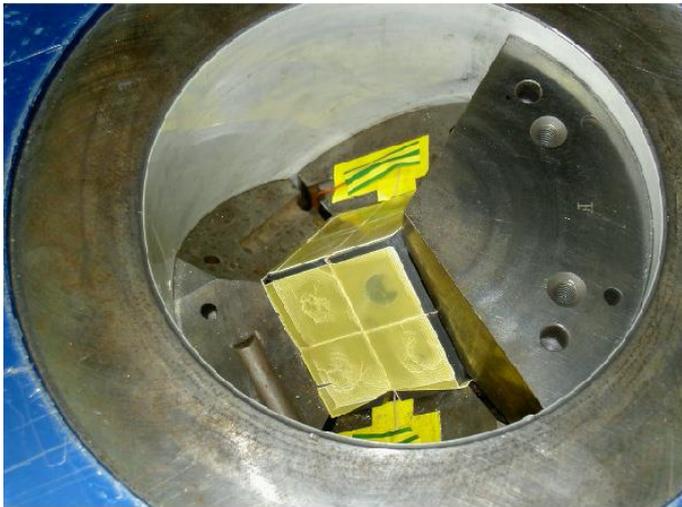


-  Octaèdre de magnésie
-  Céramique en Al_2O_3
-  Ciment
-  MgO
-  Charge
-  Molybdène
-  $LaCrO_3$
-  Oxyde de zirconium
-  Capsule de Re ou Au
-  Spirale de cuivre
-  Thermocouple

5 mm

Coupe de l'assemblage octaédrique

Forces





Press 1500 tons, Clermont Ferrand



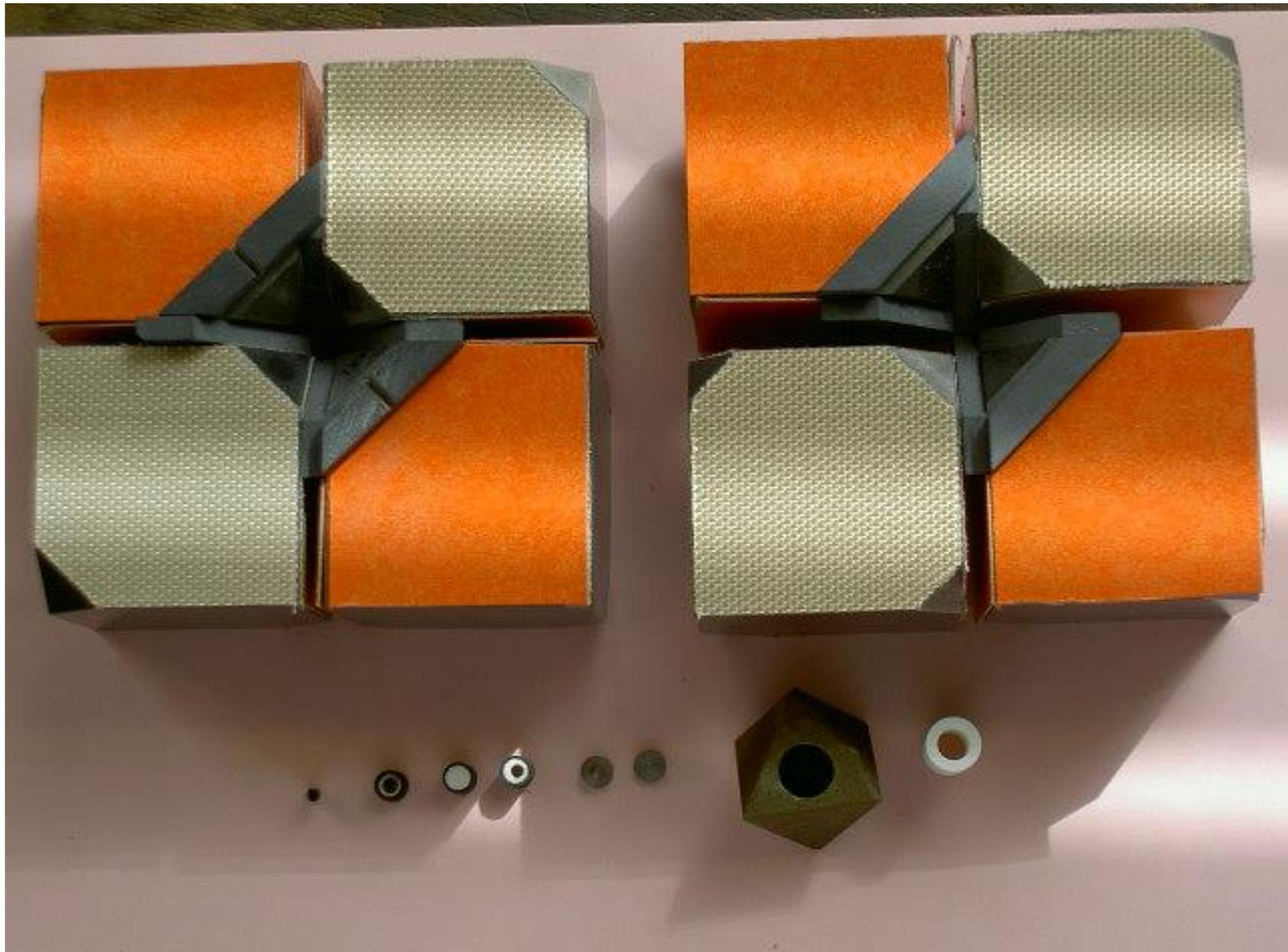
Press 5000 tons, Misasa, Japan

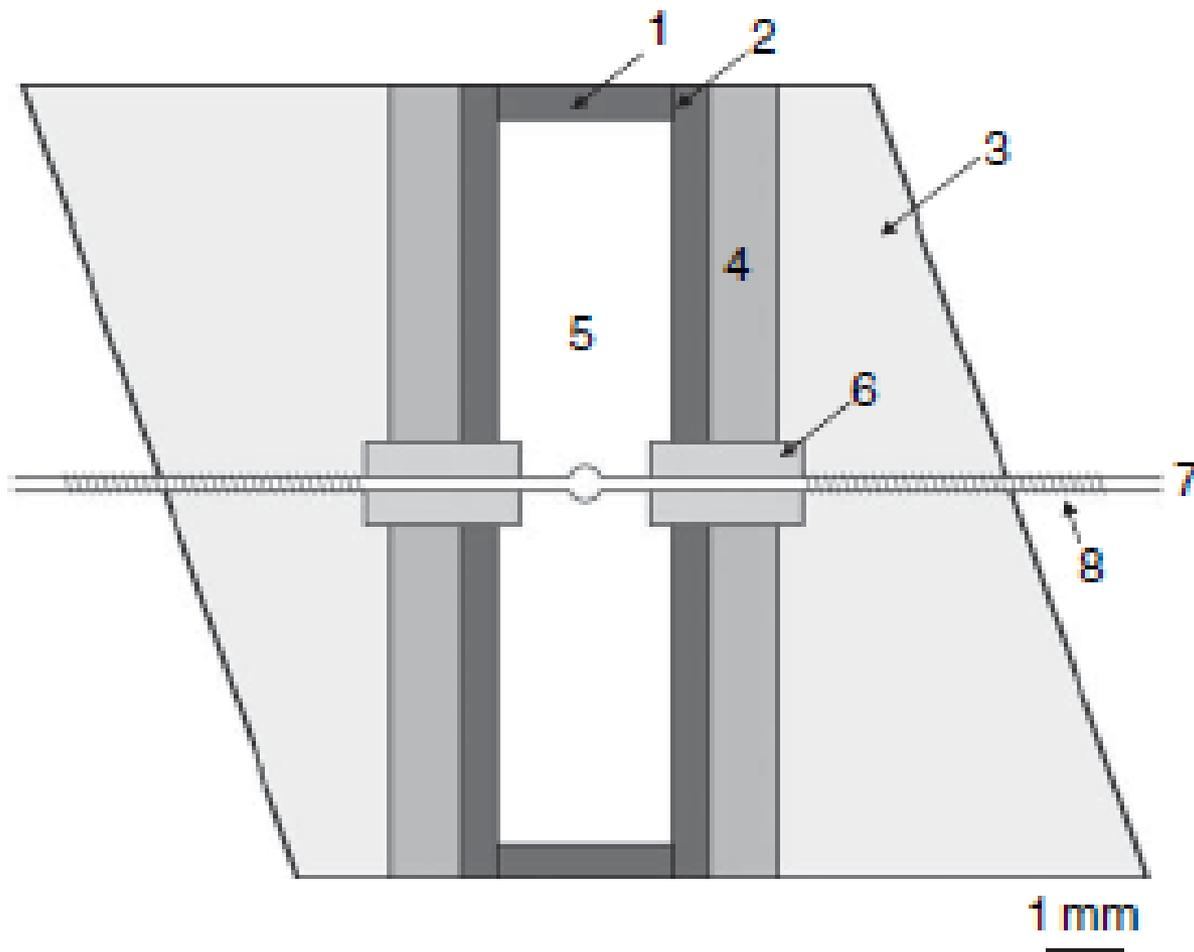


Press 6000 tons, Ehime, Japon

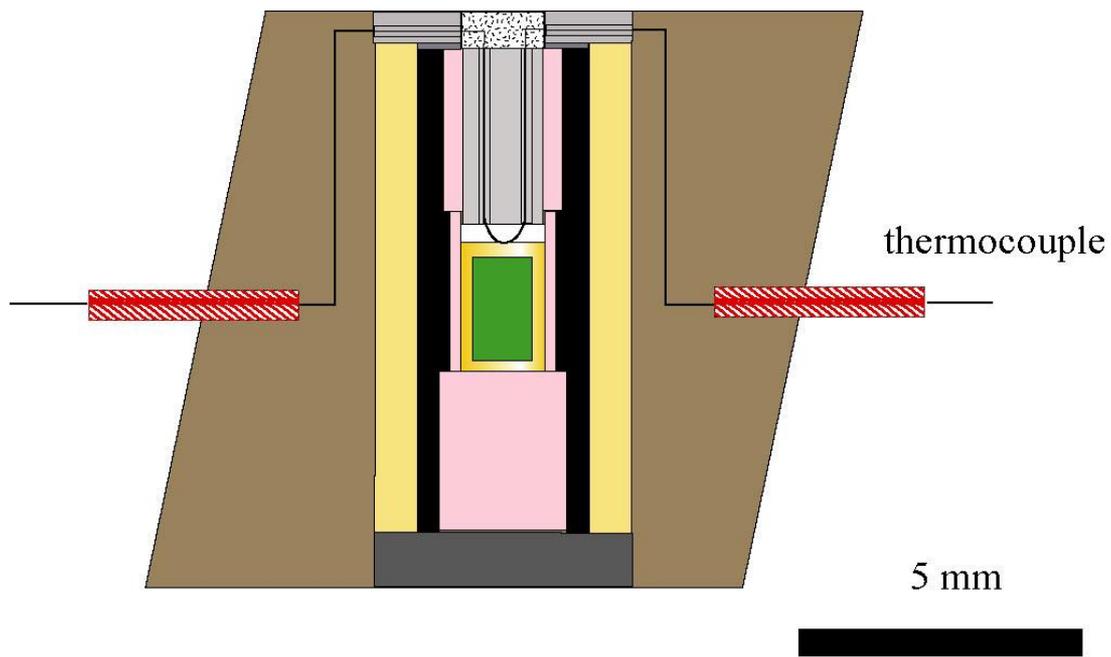


Press BARS, Novossibirsk, Russie





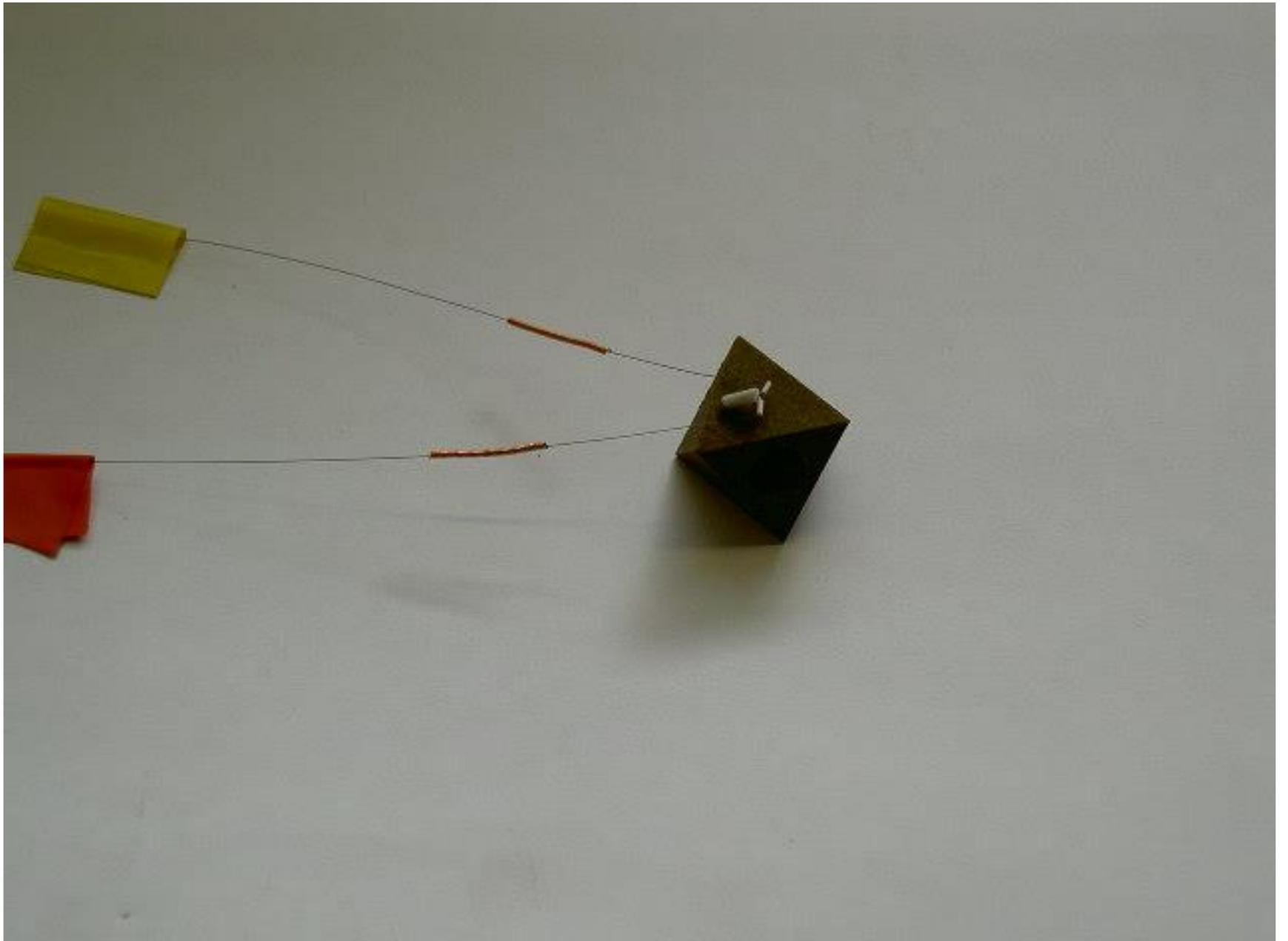
- 1: Lid; 2: Heater; 3: Pressure medium;
- 4: Thermal insulator; 5: Sample;
- 6: Electric insulator; 7: Thermocouple;
- 8: Coil

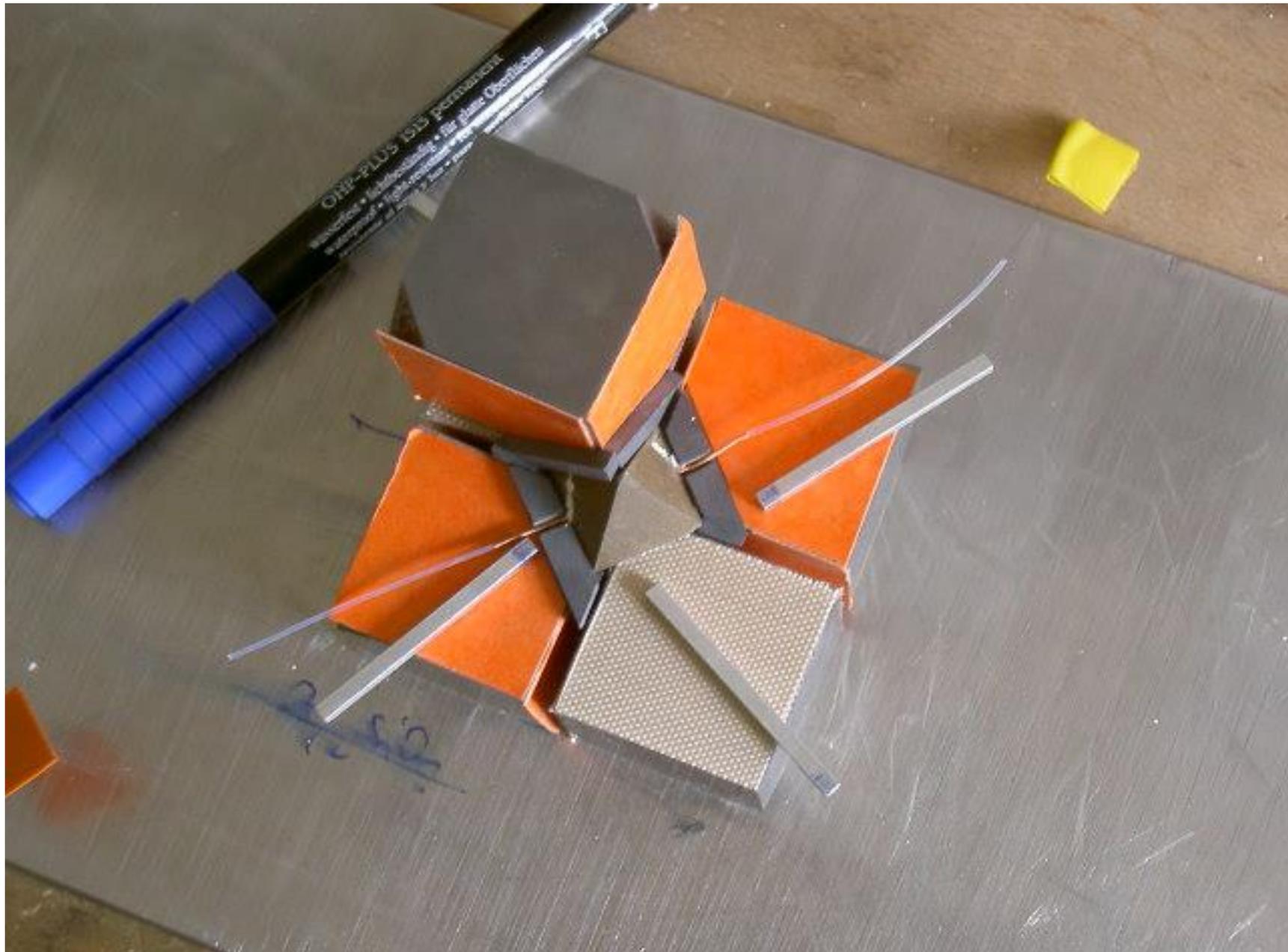


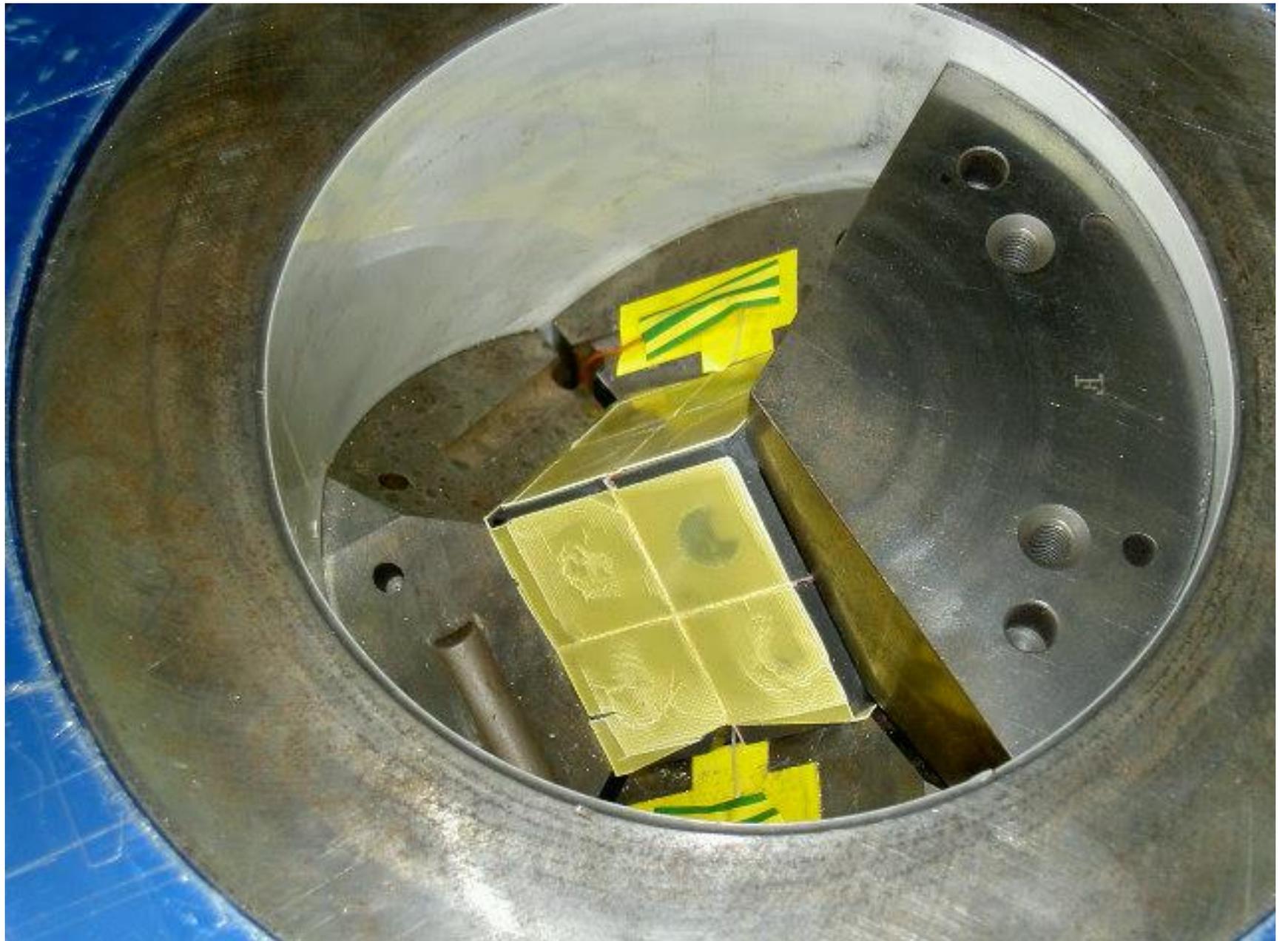
-  Octaèdre de magnésie
-  Céramique en mullite
-  Ciment
-  MgO
-  Charge
-  Molybdène
-  LaCrO₃
-  Oxyde de zirconium

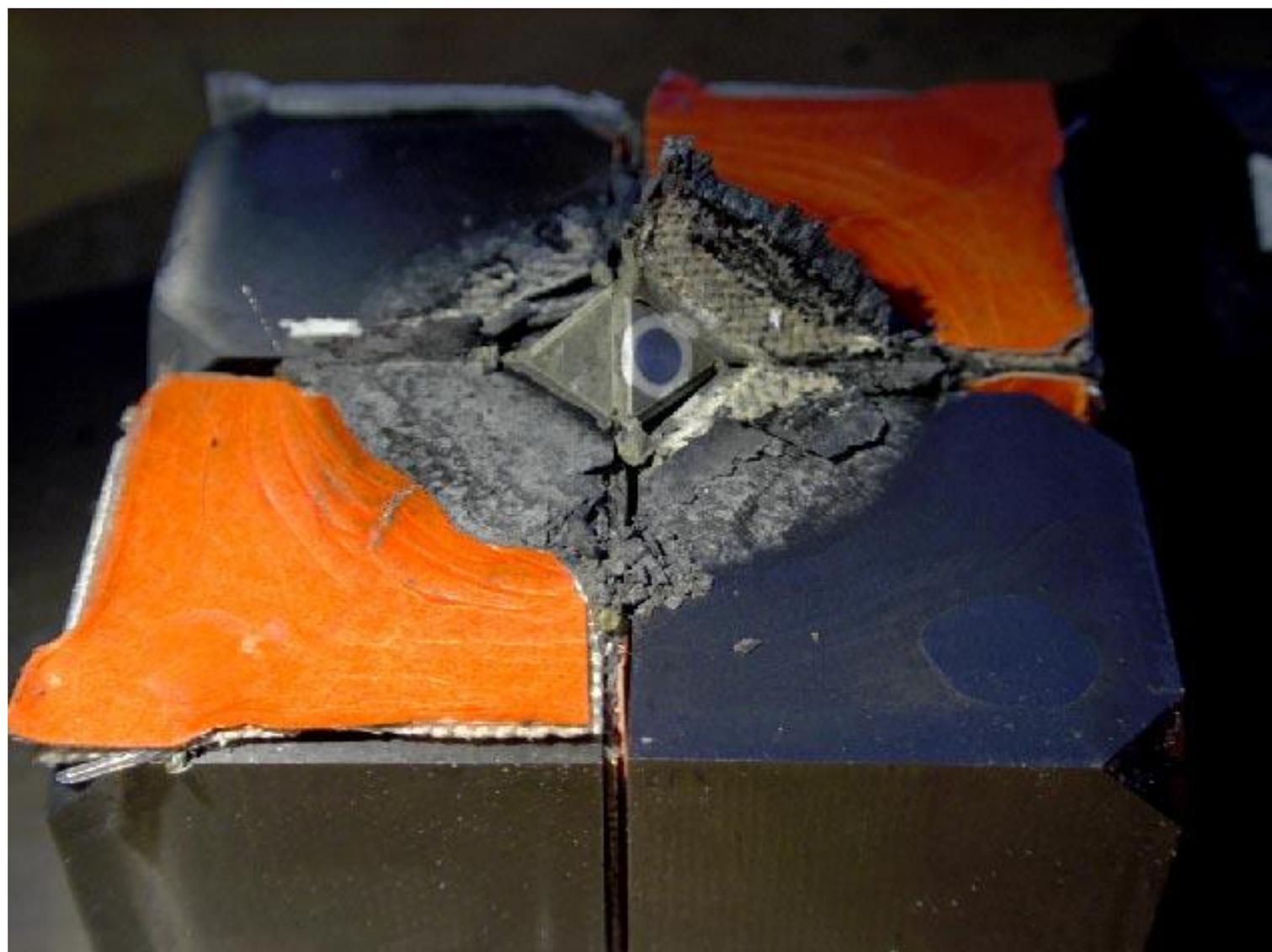
-  Capsule de Re ou Au
-  Spirale de cuivre
-  Thermocouple



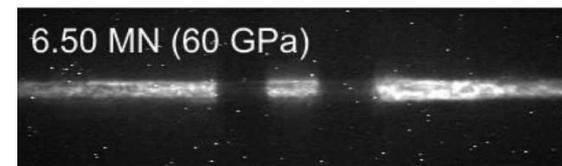
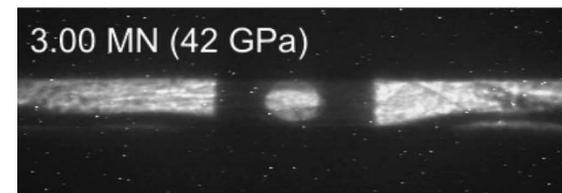
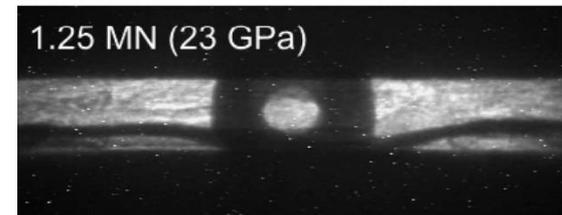
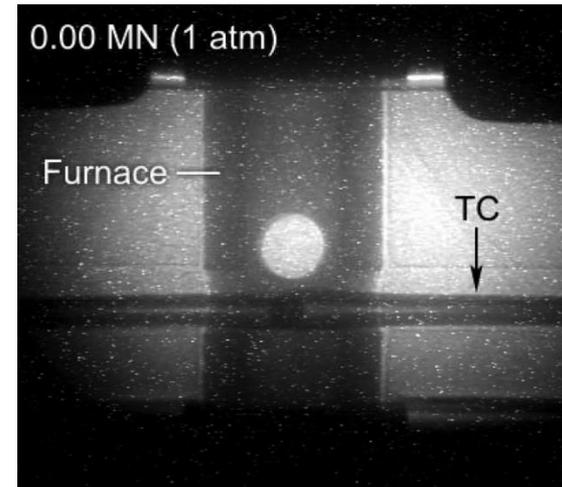
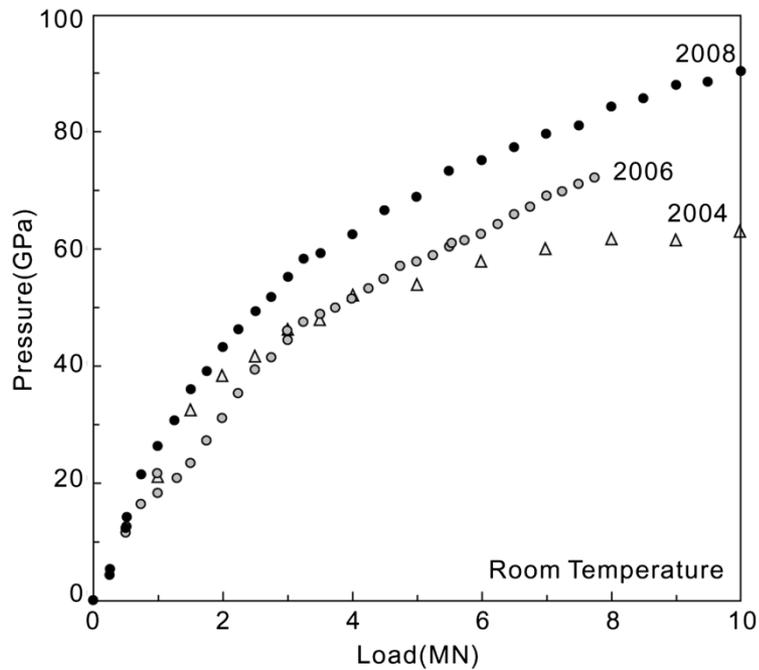
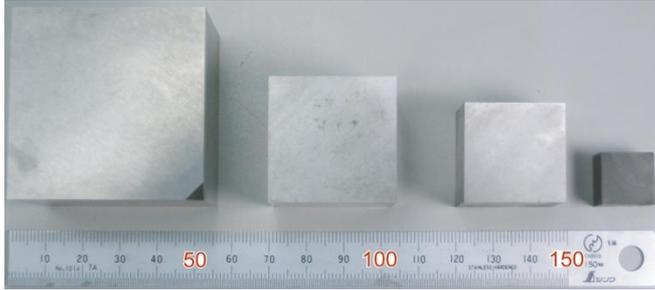






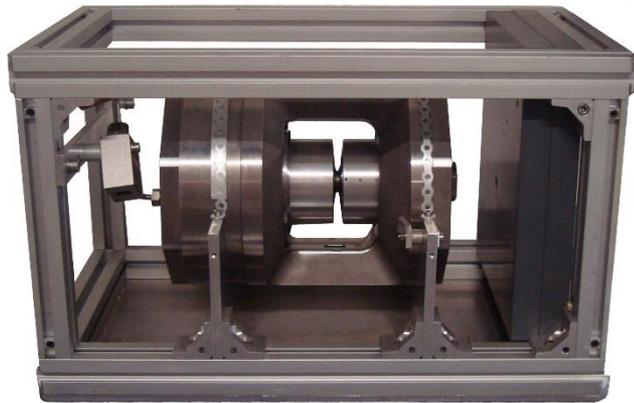


Sintered diamond anvils

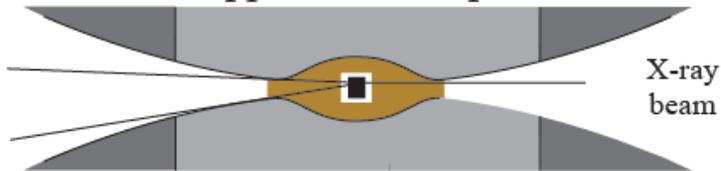


1.0 mm

Other large volume presses

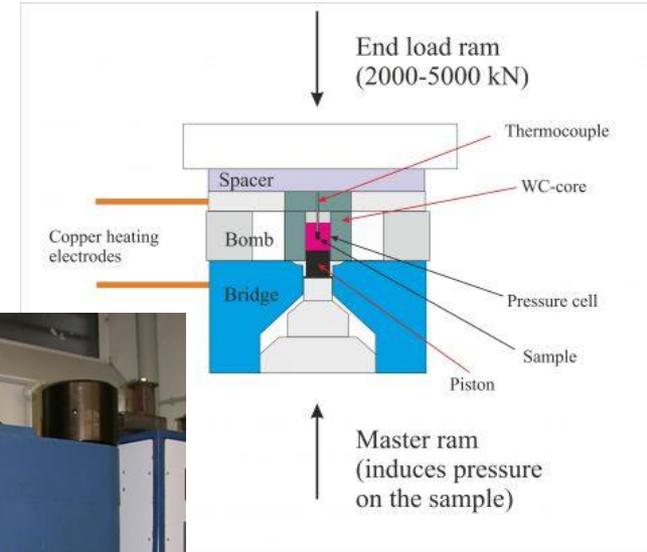


Opposed anvils press



X-ray beam

Paris-Edinburgh Press
Developped for in-situ experiments
Pressure up to ~15 Gpa
Temperature up to 2300 K

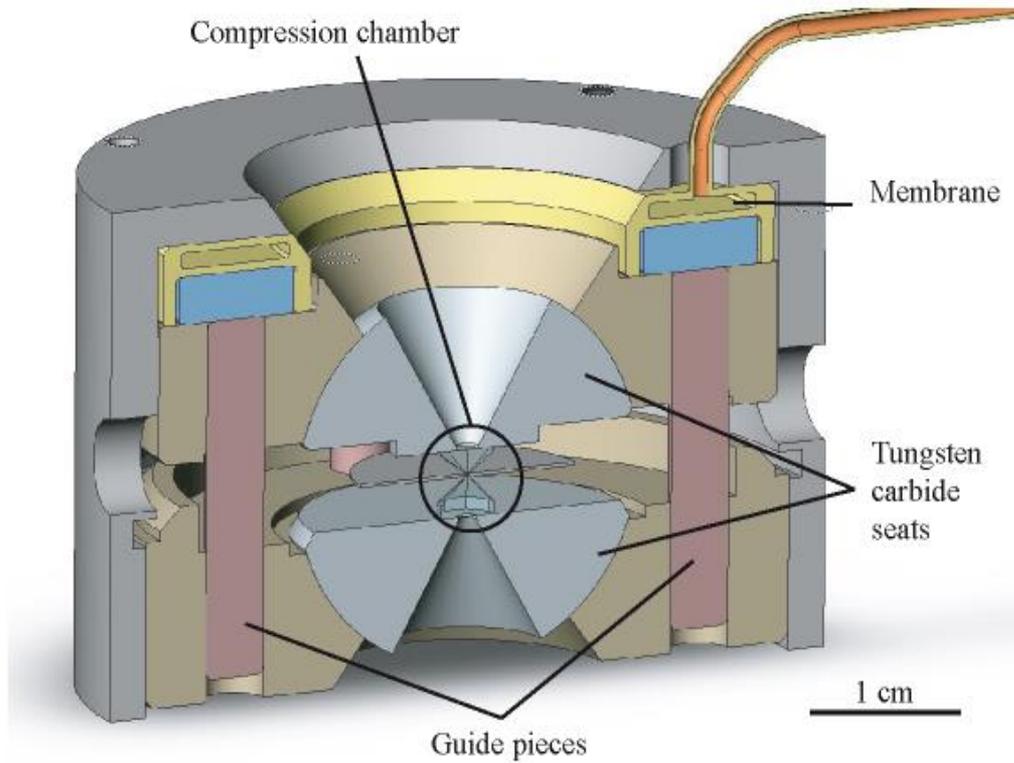


Piston cylinder apparatus
For ex situ synthesis
Pressure up to 4 Gpa
Temperature up to 2500 K

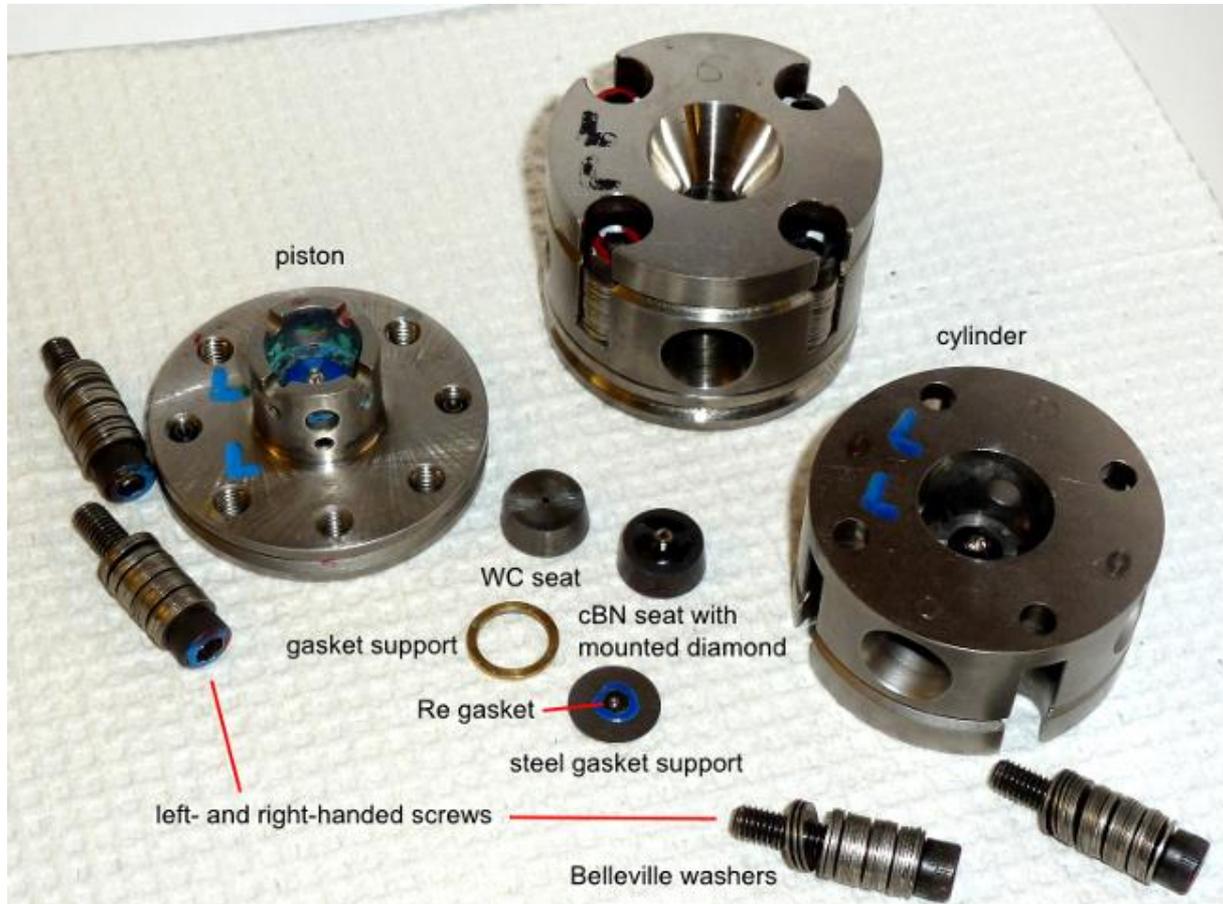
Diamond Anvil Cells

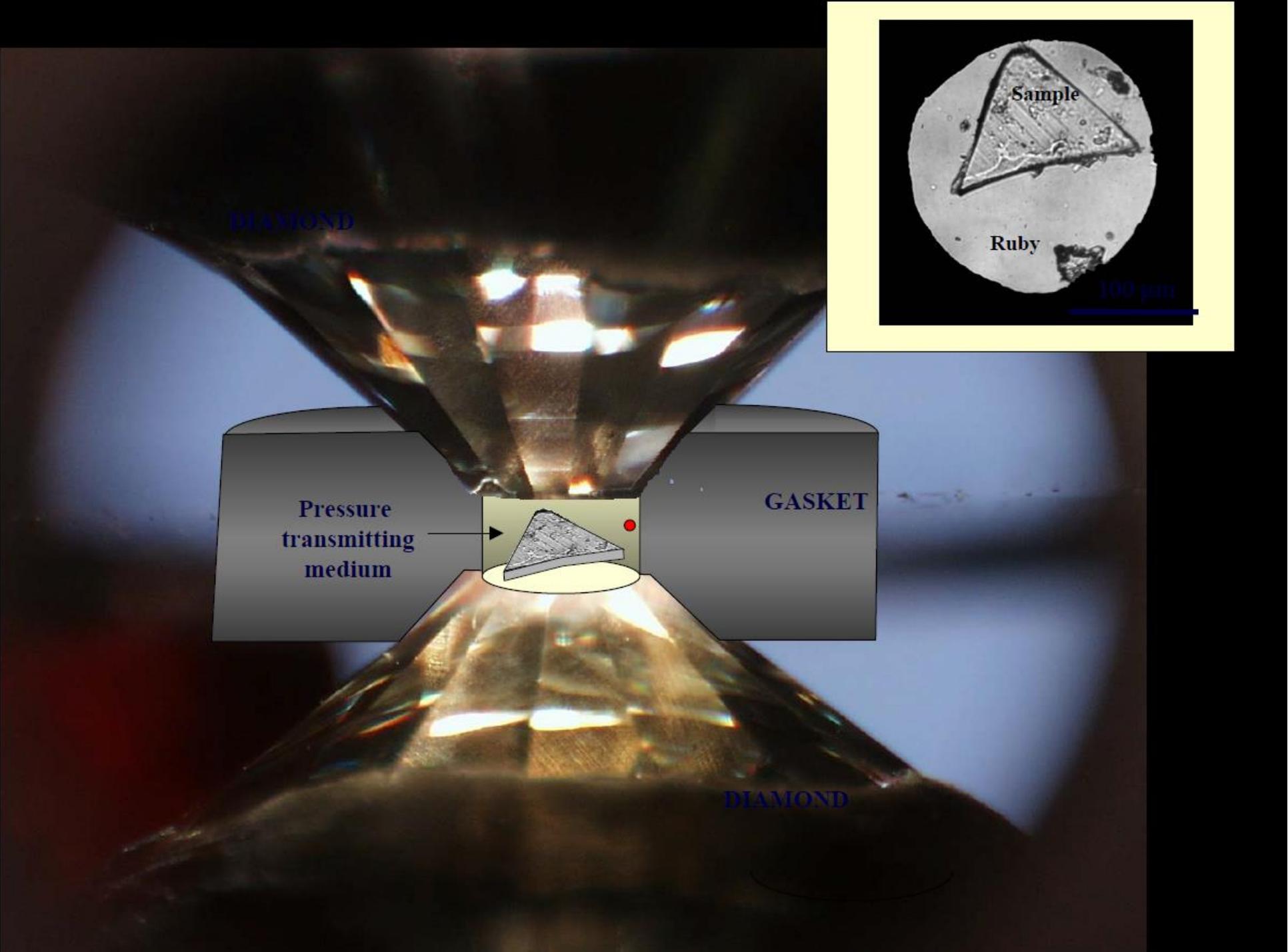
Membrane type cell

Diamond anvil cell



Mao-Type cell



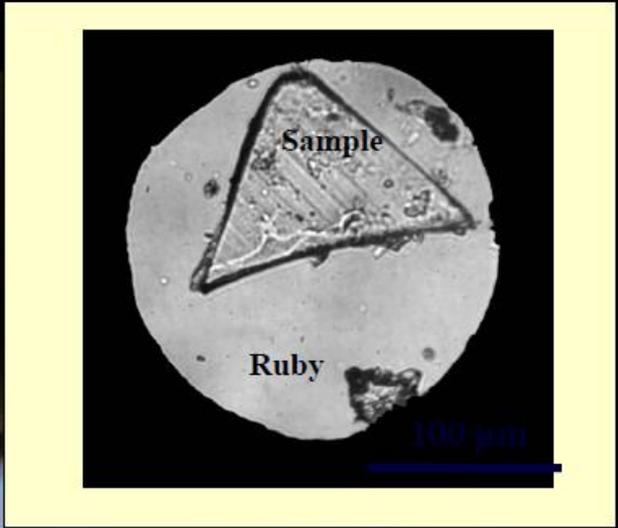


DIAMOND

GASKET

Pressure
transmitting
medium

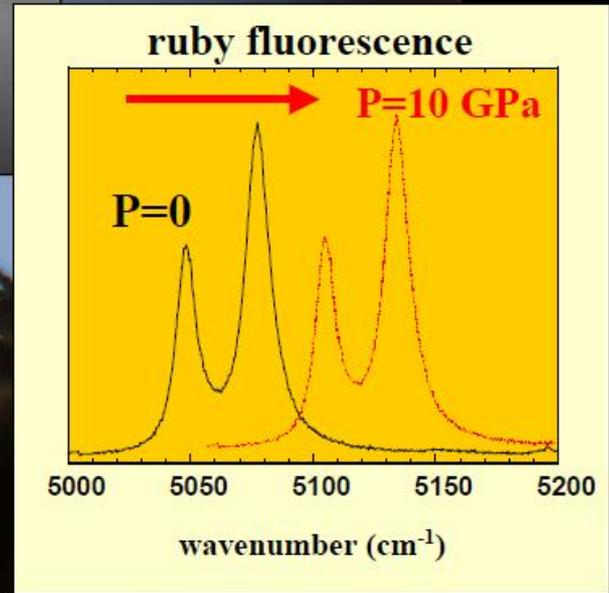
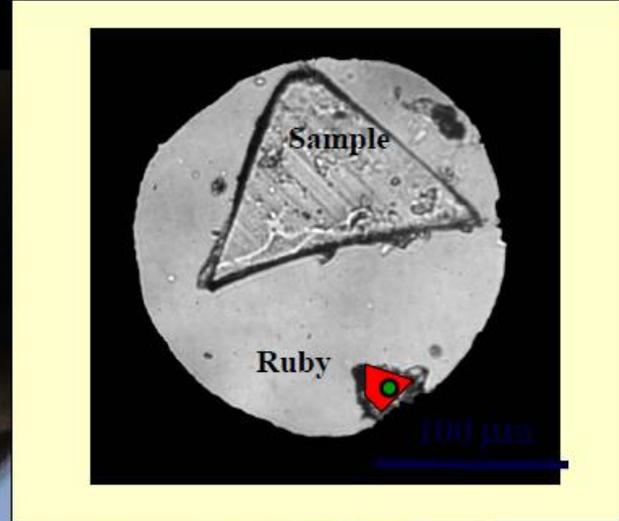
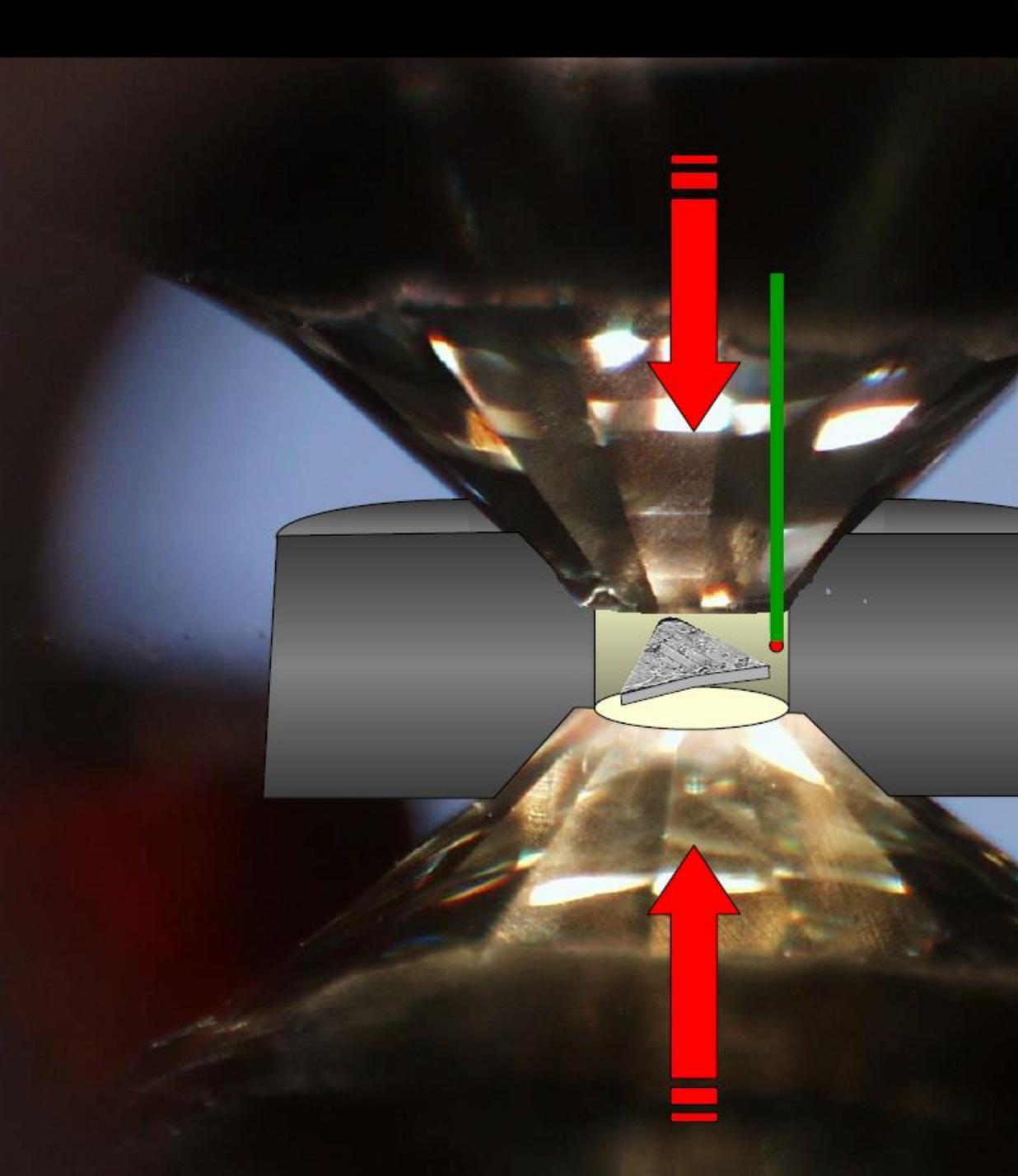
DIAMOND

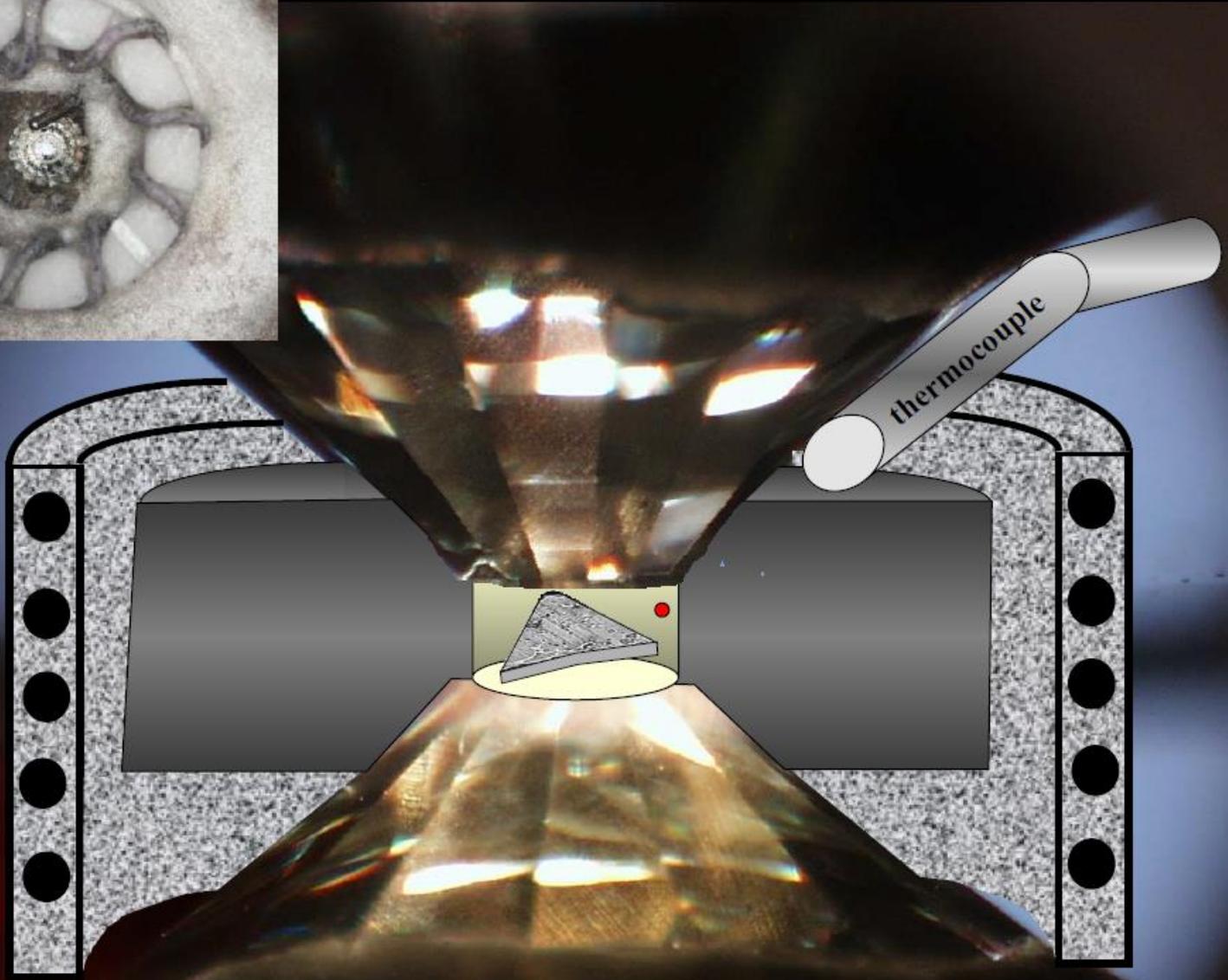


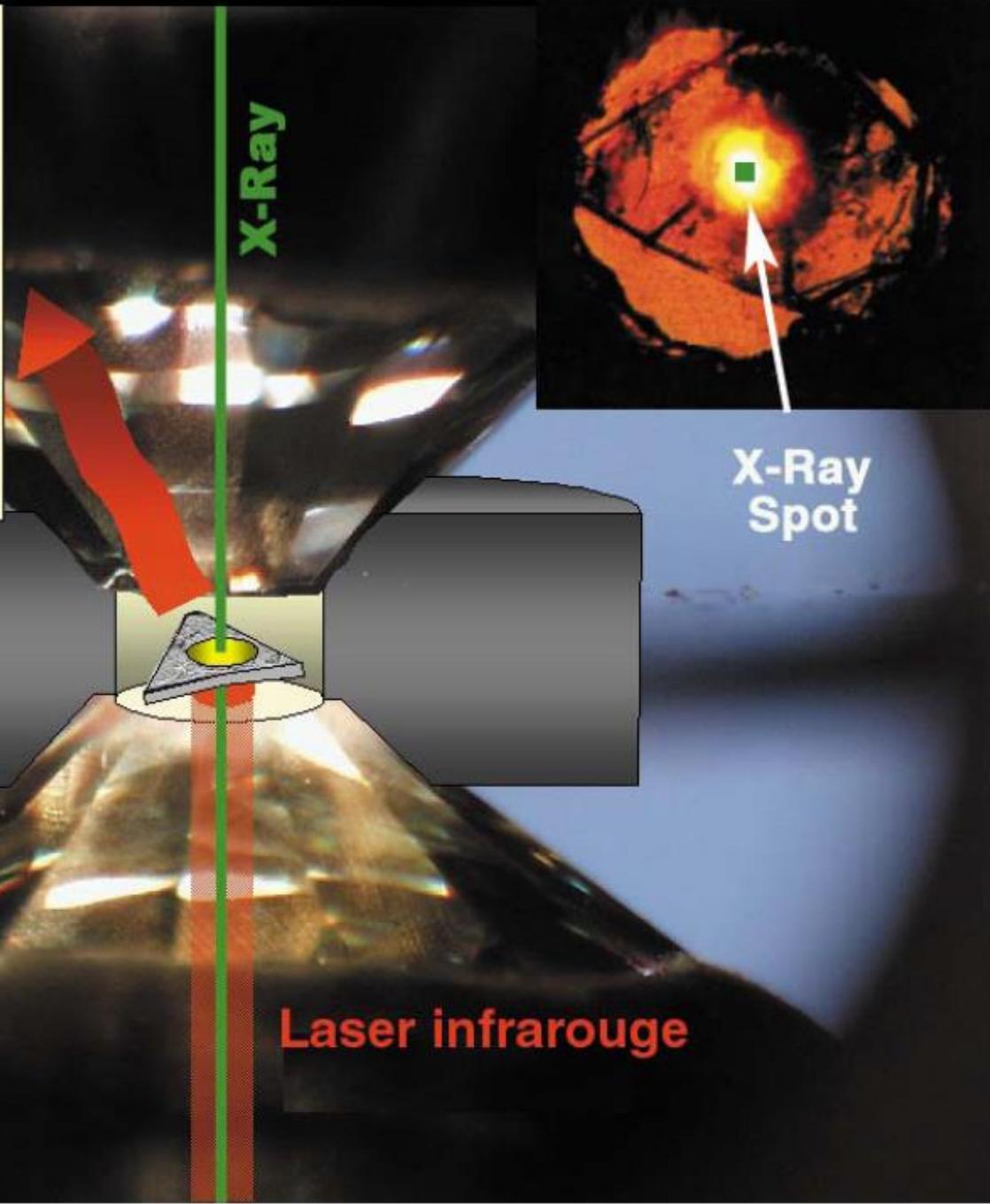
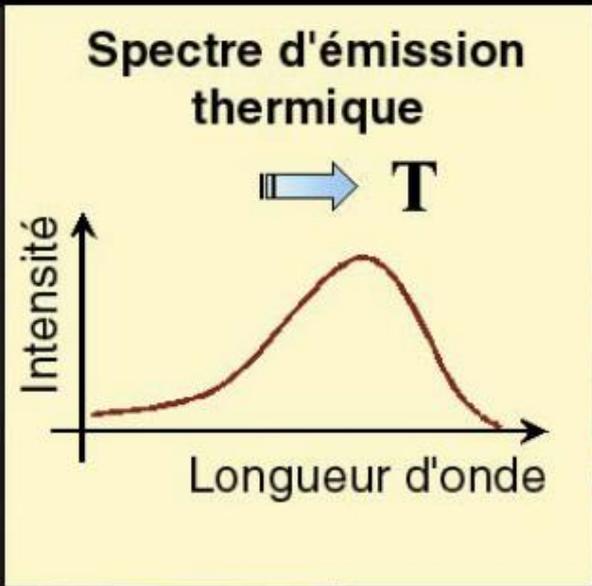
Sample

Ruby

100 μm







Double Sided Laser Heating DAC Experimental Set up

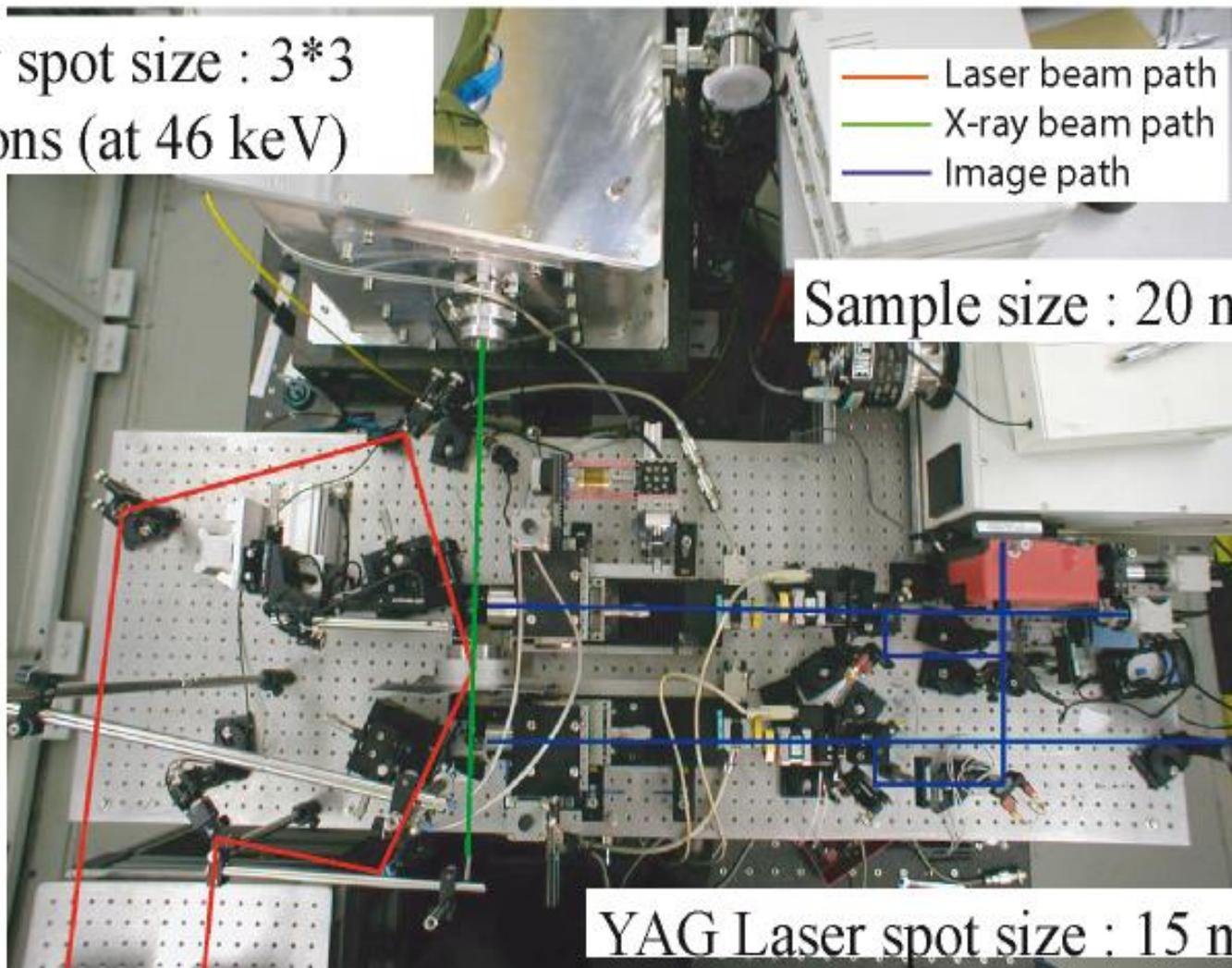
X-ray spot size : 3*3
microns (at 46 keV)

— Laser beam path
— X-ray beam path
— Image path

Sample size : 20 microns

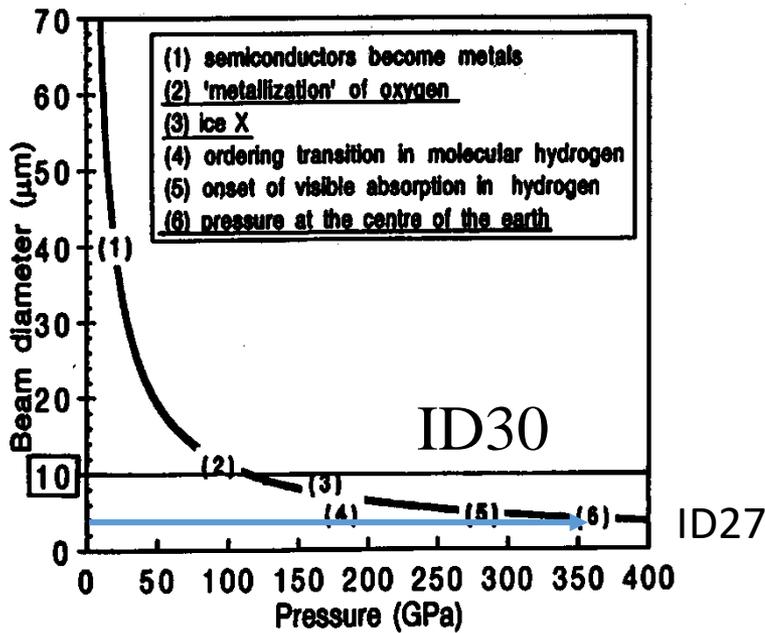
Exposure
time : 20 s

YAG Laser spot size : 15 microns

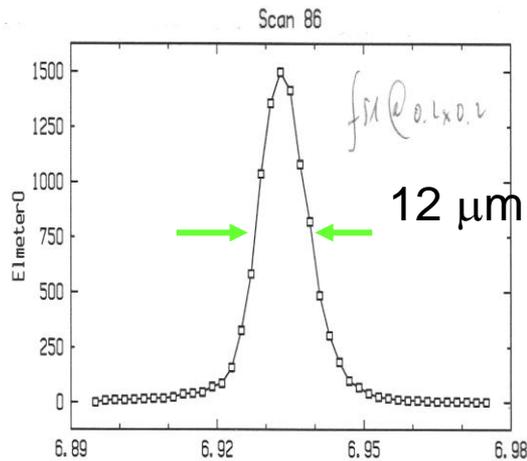


High pressure beamline at the ESRF

Change in the beamsize and in the X-ray flux

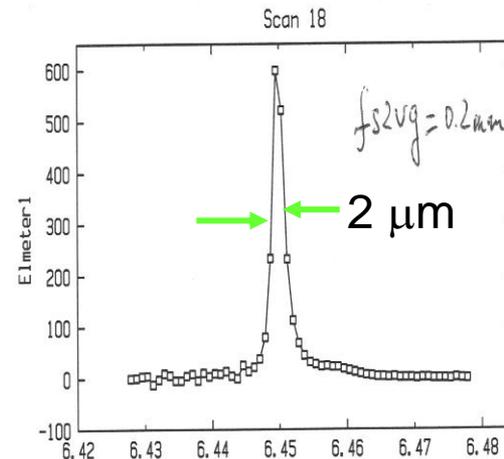


1997-2005
ID30



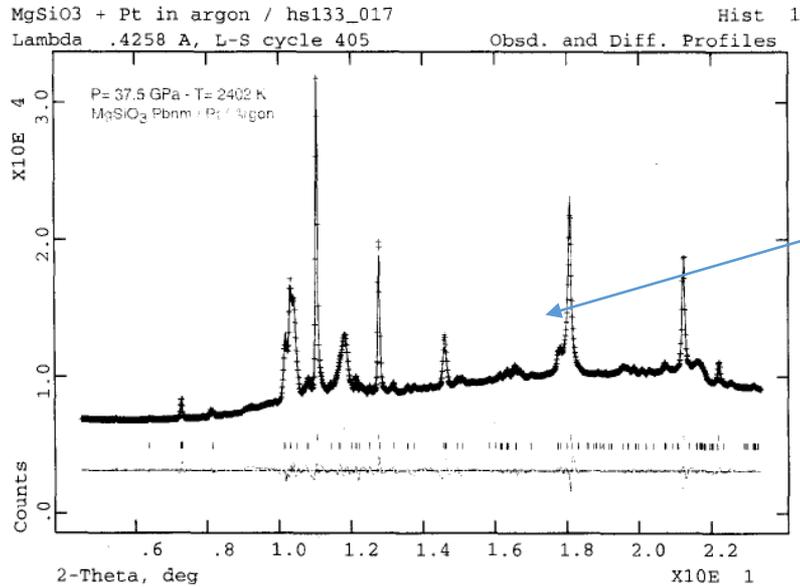
Peak at 6.9336 is 1437. CUM at 6.9333
FWHM is 0.011693 at 6.9336.

Since 2006
ID27

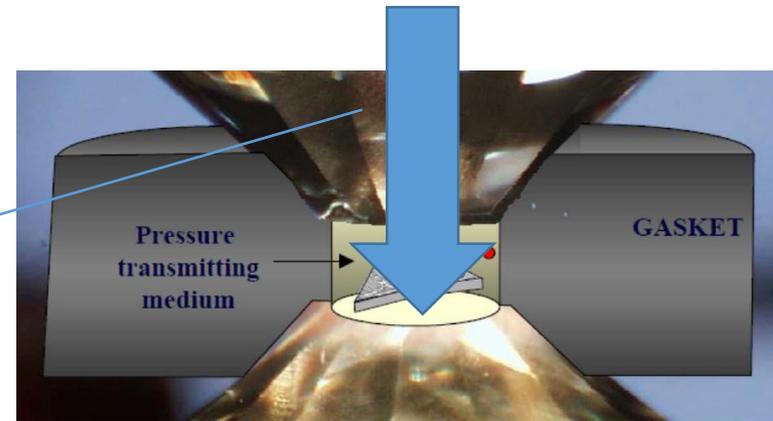


Peak at 6.4499 is 599. CUM at 6.4507
FWHM is 0.0021535 at 6.4499.

Fiquet et al, PEPI, 1998

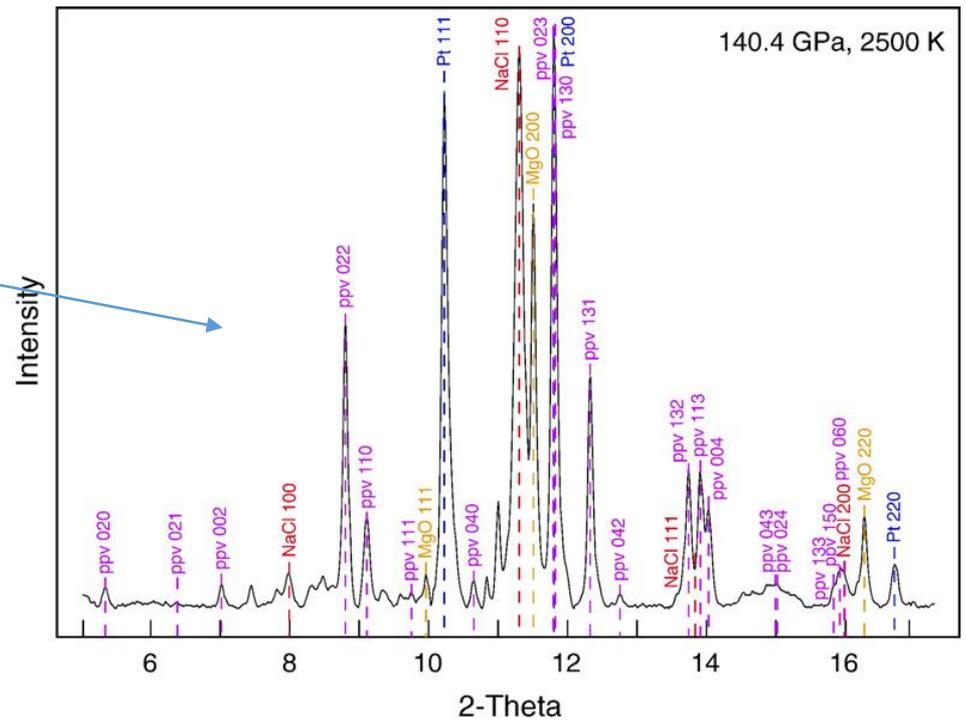
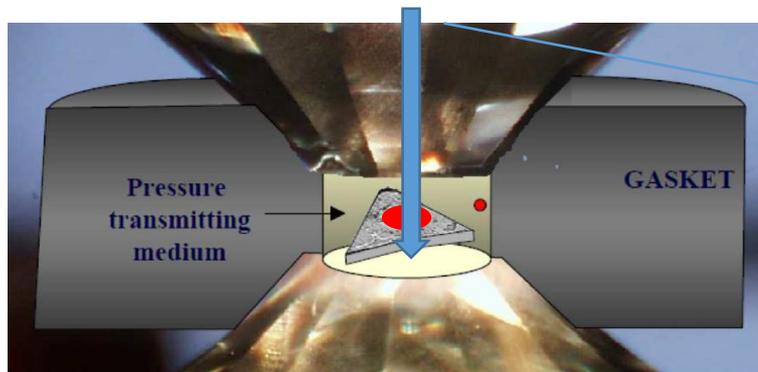


X-ray 1998

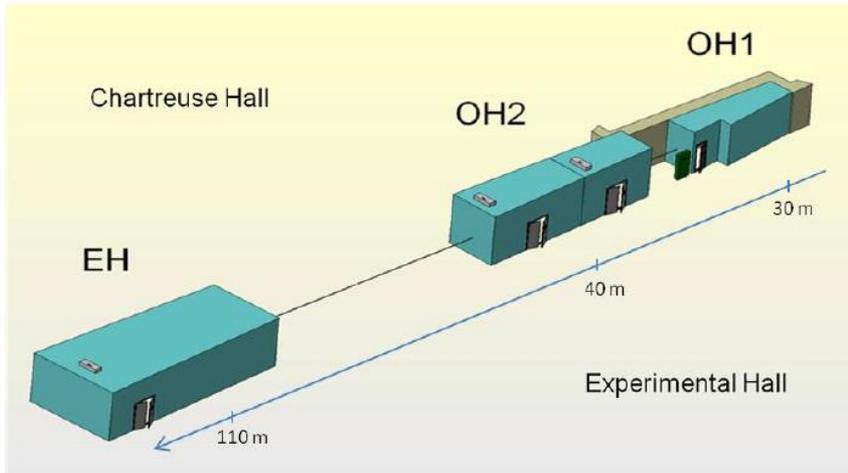


Guignot et al, EPSL, 2007

X-ray, 2007



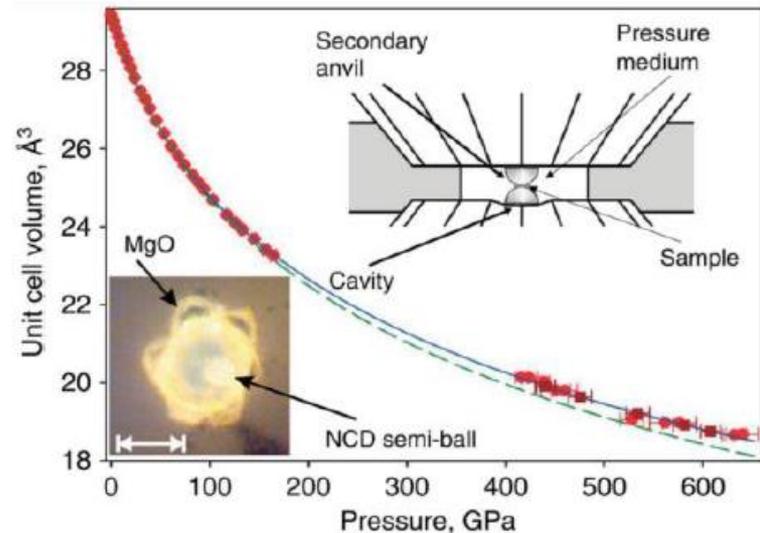
ESRF upgrade : new ID27 beamline



200 * 300 nm beam
Planned in September
2021

Over 1 000 Gpa using
Diamond Anvil Cell

Double-stage diamond anvil cell



Dynamic compression experiments

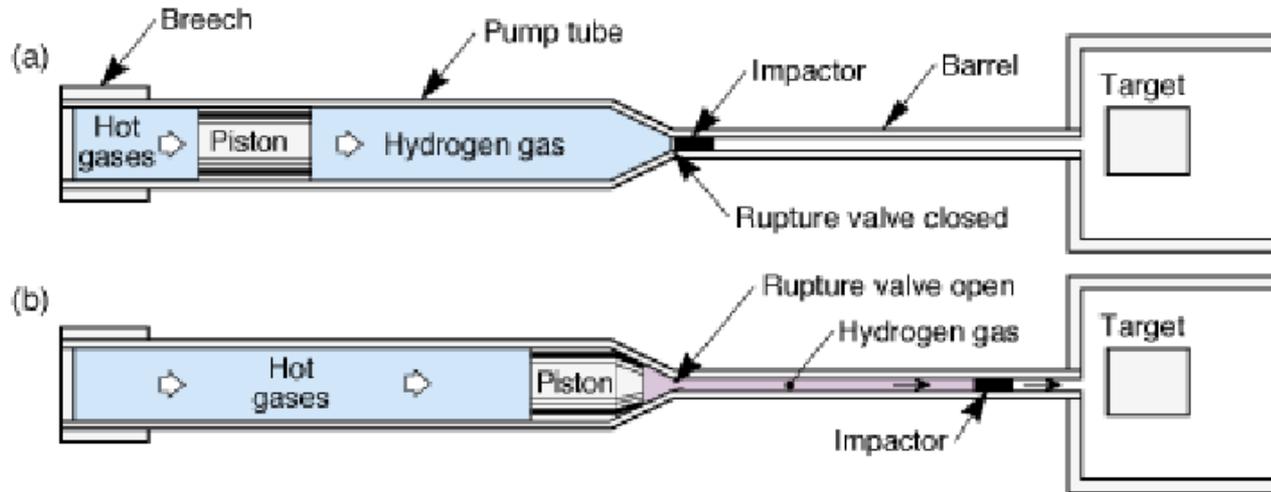
Different ways to generate a shock

Explosive set-up



Different ways to generate a shock

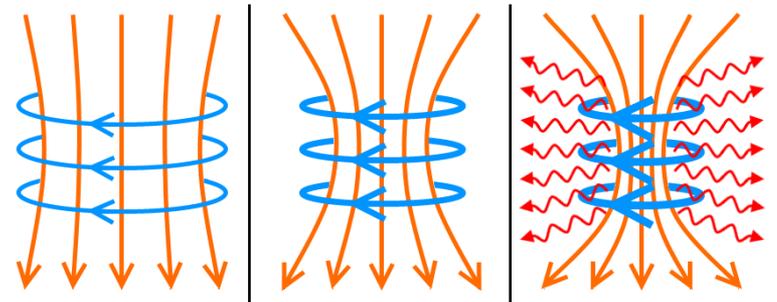
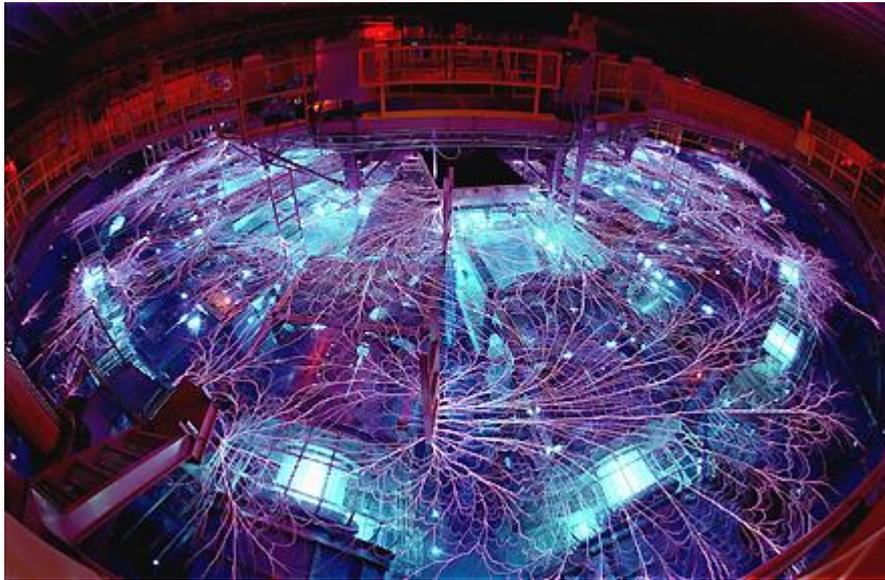
Gas-gun experiments



From Lawrence
Livermore National
Laboratory website

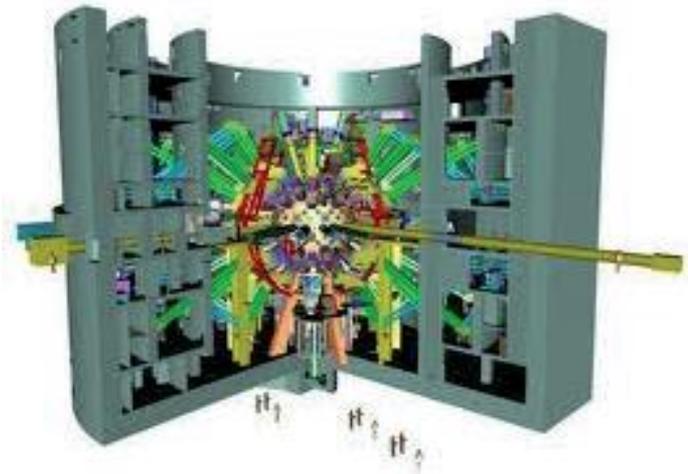
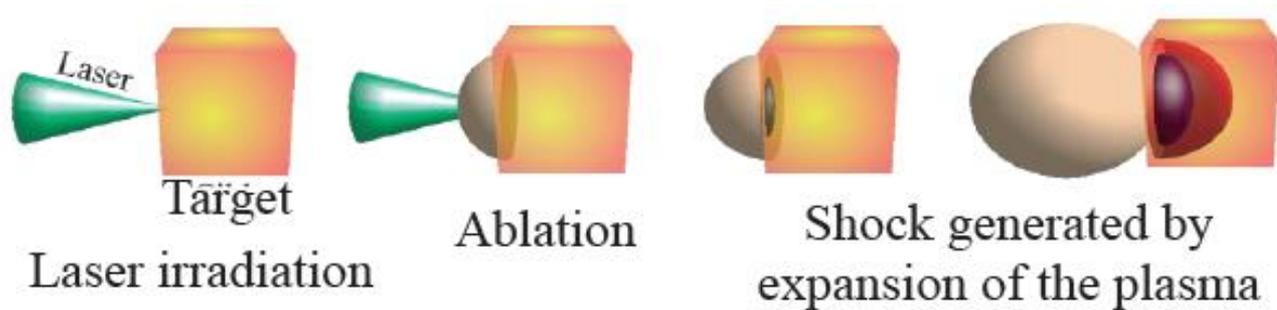
Different ways to generate a shock

Z-pinch experiments



Different ways to generate a shock

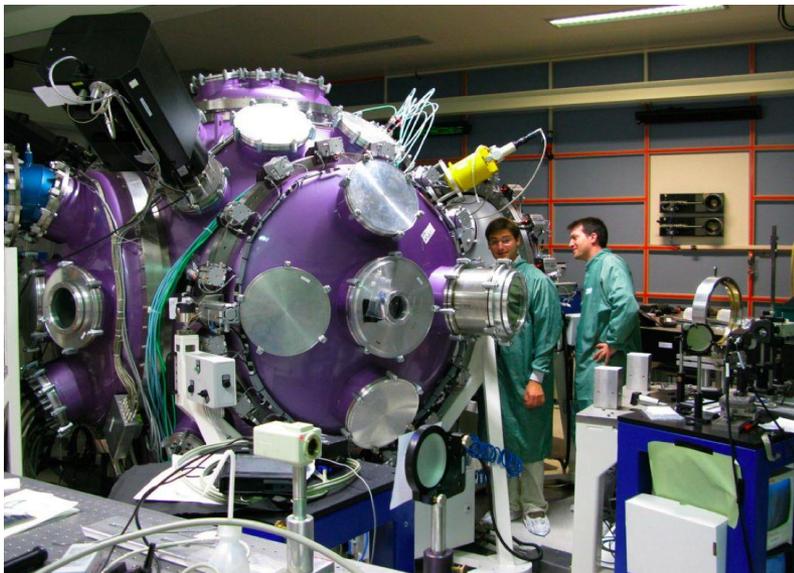
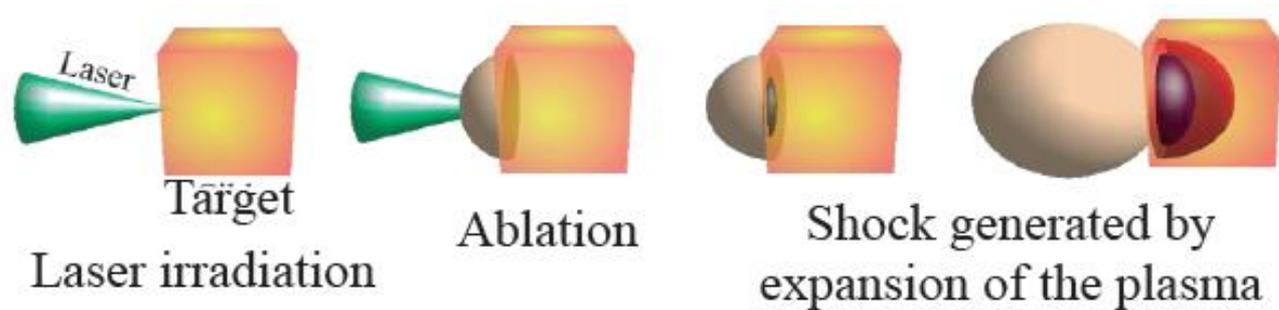
Laser shock experiments



One example : MegaJoule laser, under construction, Bordeaux, France

Different ways to generate a shock

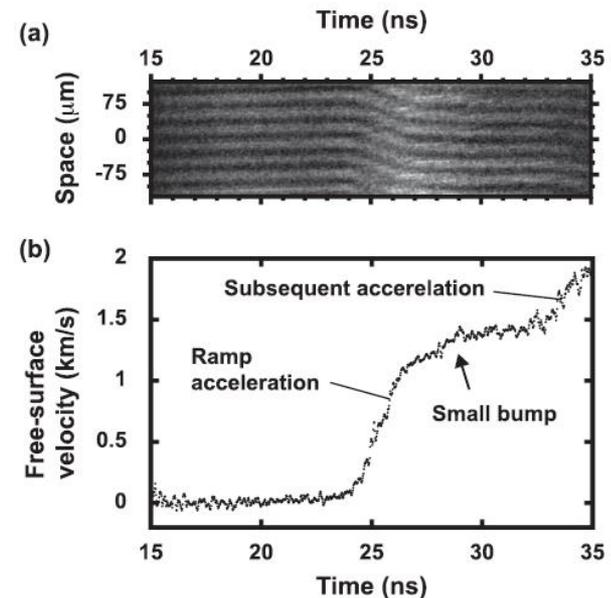
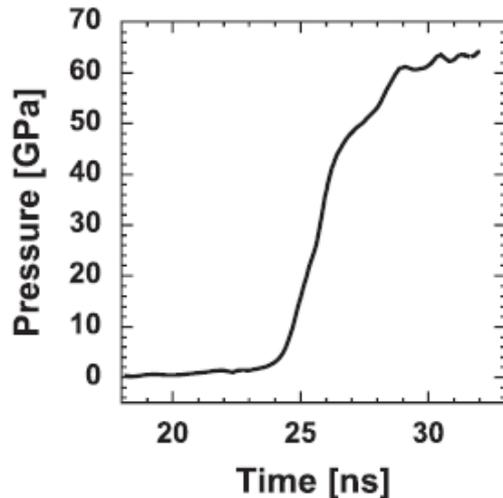
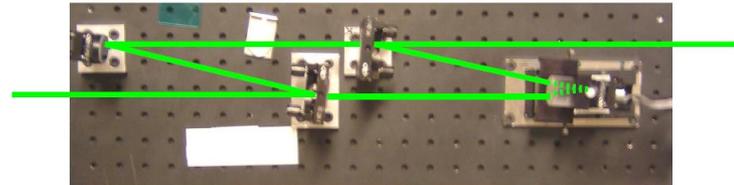
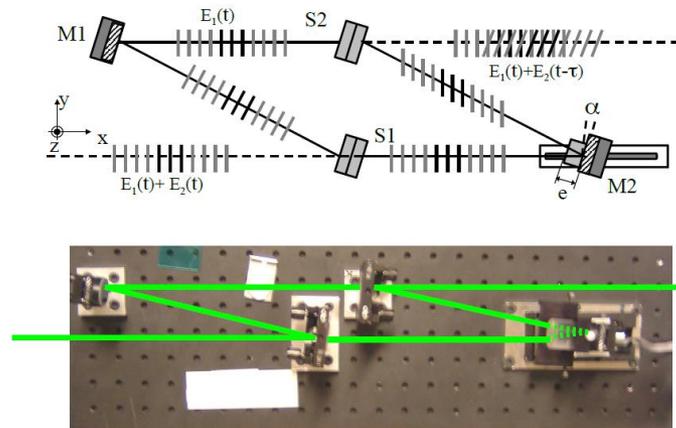
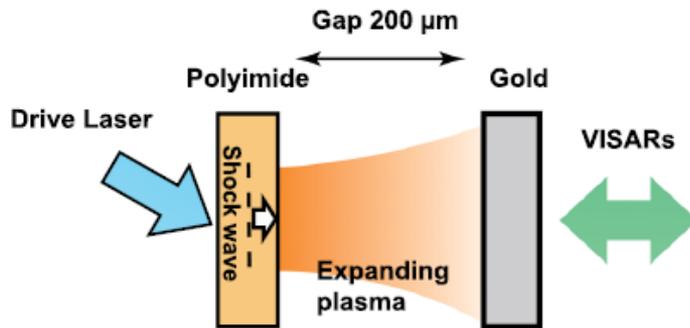
Laser shock experiments



LULI 2000, Ecole
Polytechnique,
Palaiseau, France

Casual diagnostic in shock experiments

Velocity Interferometer for Any Reflector (VISAR)



From Miyanishi et al, *J. App. Phys.*, 2014

Casual diagnostic in shock experiments

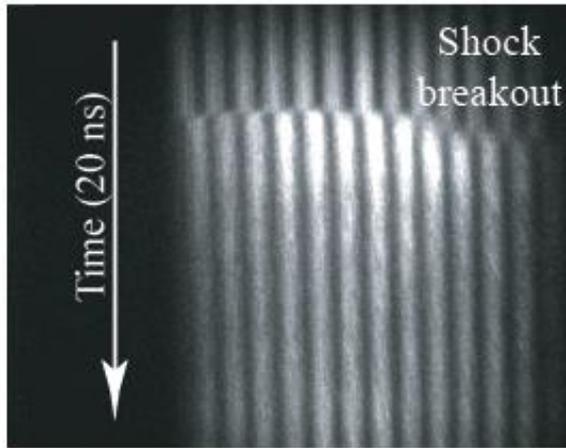
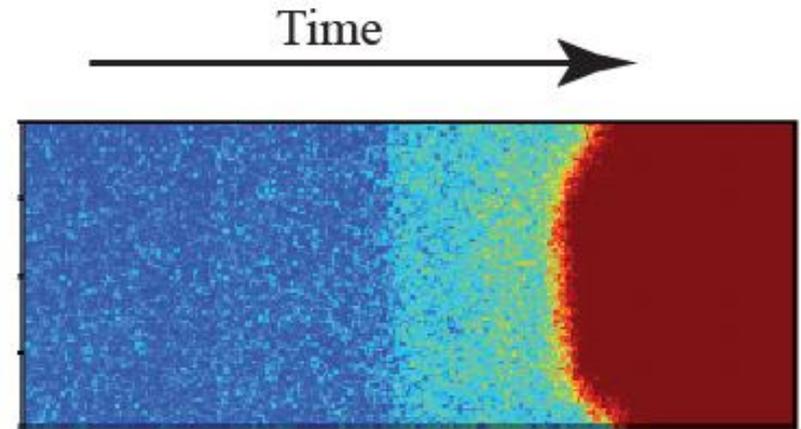


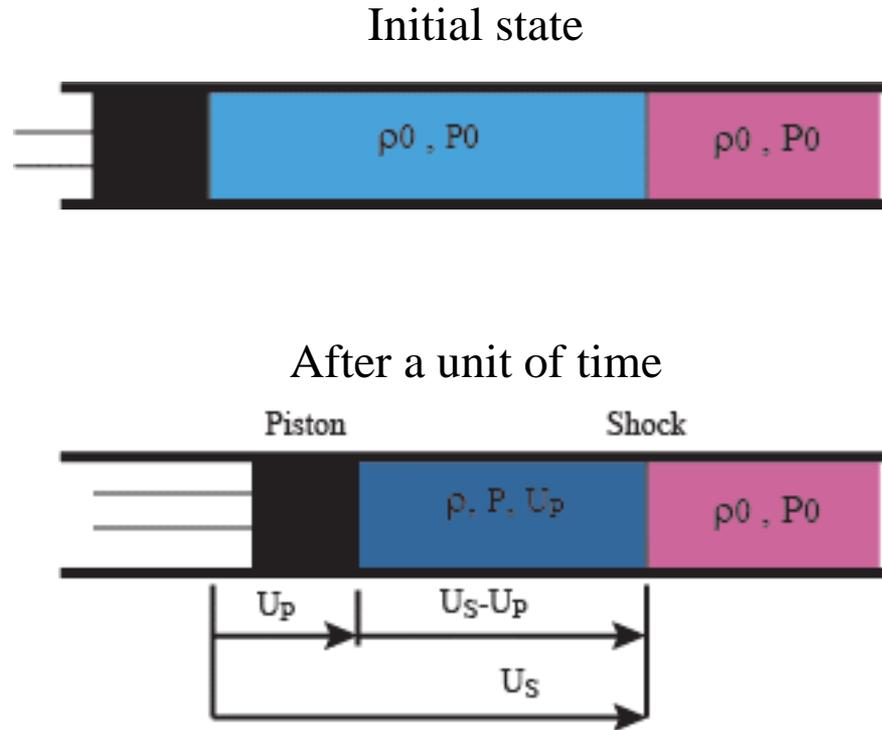
Image of interferometry of the rear face (VISAR)
Related to the pressure



Streaked Optical Pyrometer
Related to the temperature

VISAR + SOP +.... X-ray diagnostics !!!

The conservation laws for a single shock

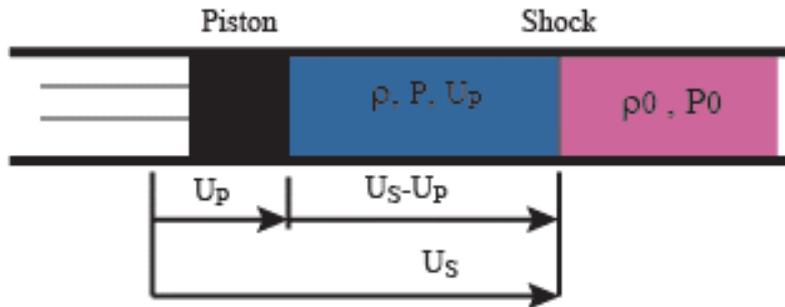
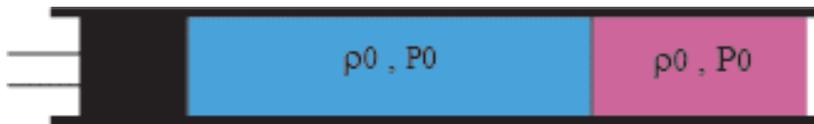


U_p : Piston
velocity
 U_s : Shock front
velocity
 A : Piston surface

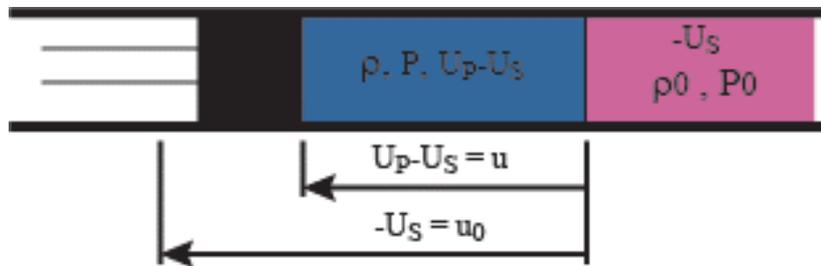
The conservation laws for a single shock

The Rankine-Hugoniot equations

Initial state



Shock fixed coordinates



- Conservation of mass

$$\rho u = \rho_0 u_0$$

- Conservation of momentum

$$p + \rho u^2 = p_0 + \rho_0 u_0^2$$

- Conservation of energy

$$\frac{p}{\rho} + e + \frac{1}{2}u^2 = \frac{p_0}{\rho_0} + e_0 + \frac{1}{2}u_0^2$$

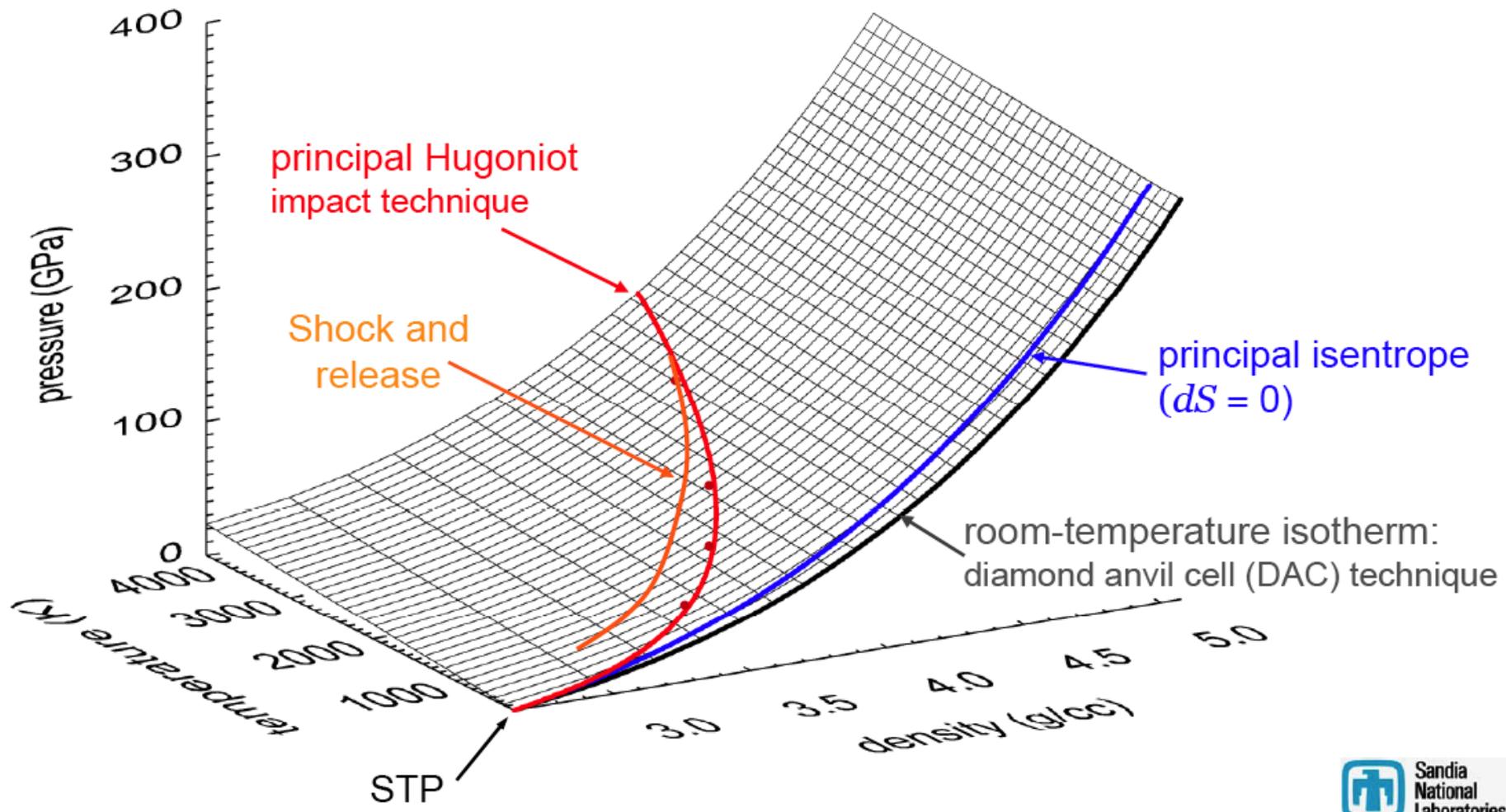
The Hugoniot equation

By removing velocities from the Rankine-Hugoniot equations,
we obtain the Hugoniot equation

$$e - e_0 = \frac{1}{2}(P + P_0) \left(\frac{1}{\rho_0} - \frac{1}{\rho} \right) = \frac{1}{2}(P + P_0)(V_0 - V)$$

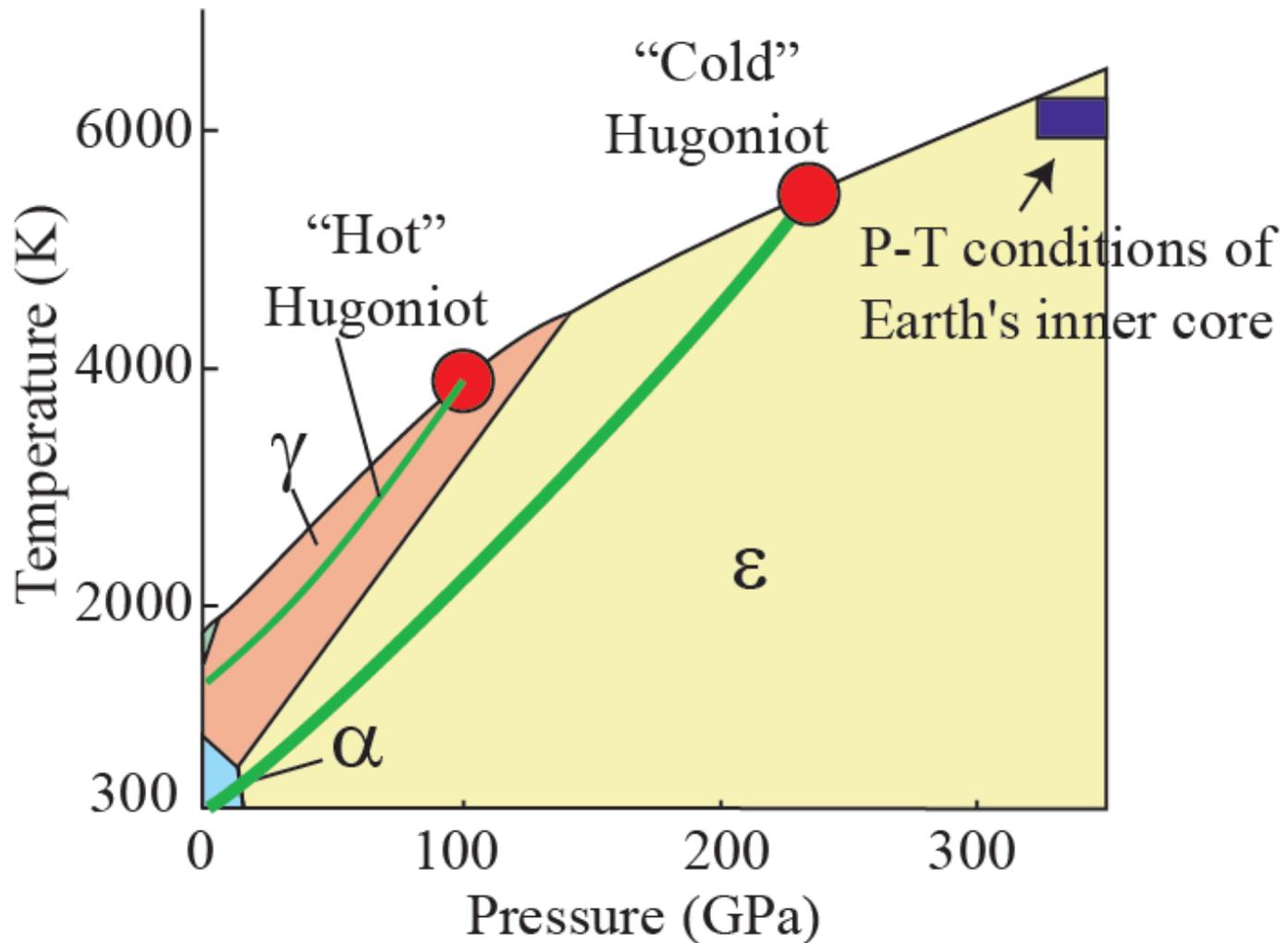
1- In the (P, ρ) space, the Hugoniot equation defines a line of possible state during the shock

2- Thermodynamic of the shock strongly depends on initial conditions (P_0, V_0)

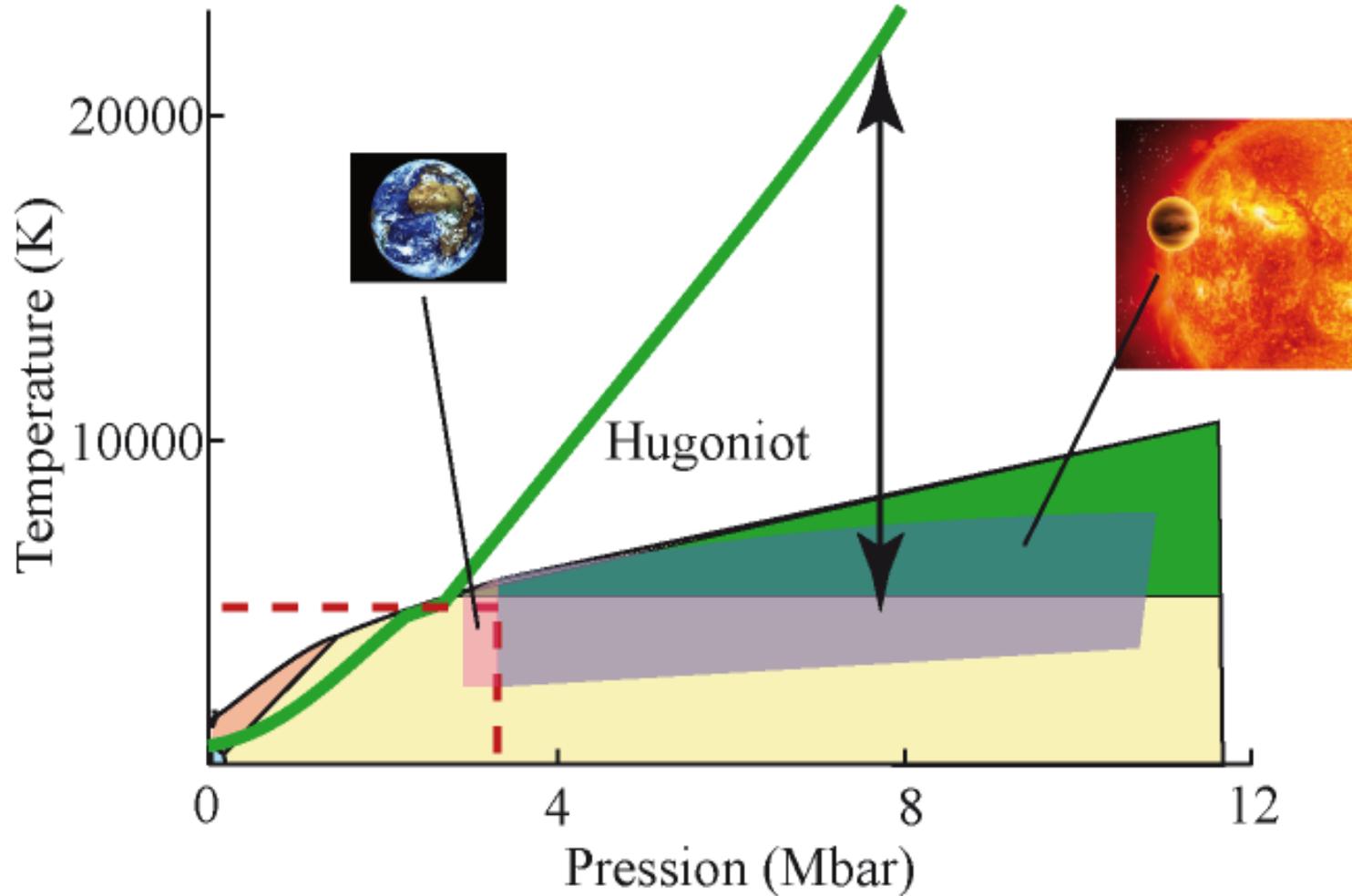


P, V, T path during shock experiments

Shock experiments on iron



Iron phase diagram under exoplanets' core conditions



A complementary technique to probe iron under extreme conditions



Experiments



Calculations

Molecular dynamics calculations

Molecular dynamics calculations
performed using ABINIT code

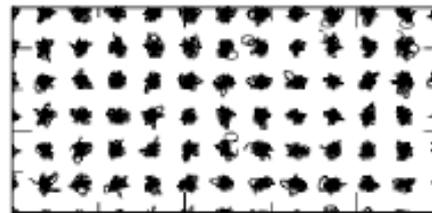
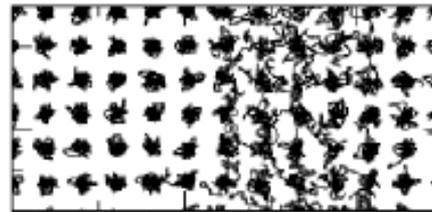
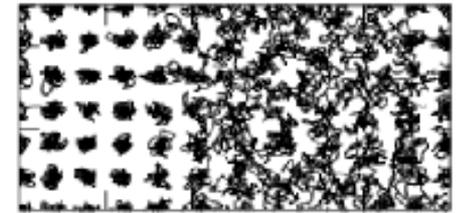
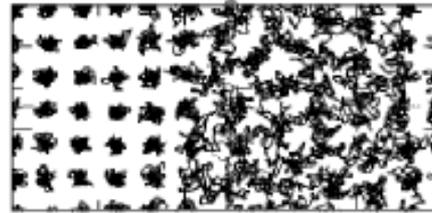
PAW method for calculation of
electronic structure

The electrons are treated
quantum mechanically
using the DFT

GGA method for the exchange-
correlation energy and potential

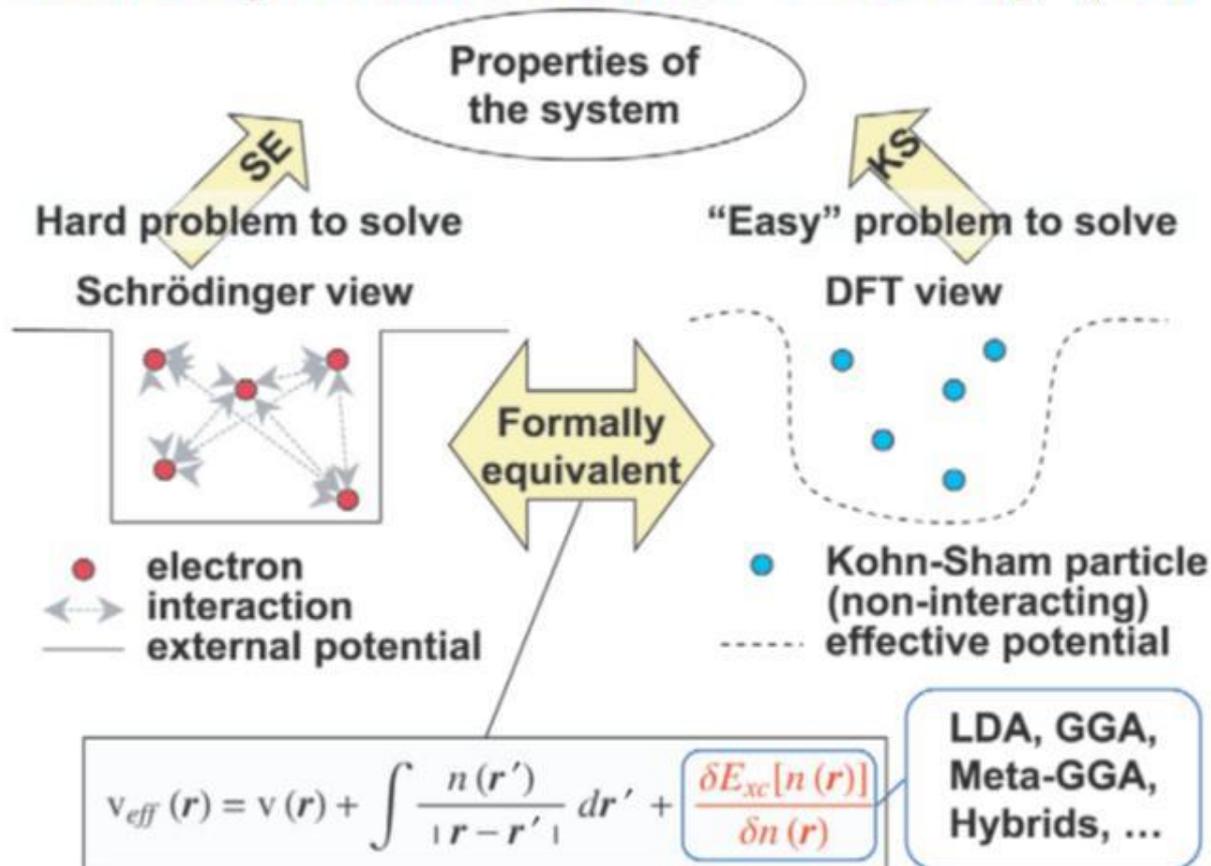
NVT method

256 atoms



Pure Fe melting temperature
calculated using the
coexistence method

Density Functional Theory (DFT)



Mattsson, et al., *Simulation in Materials Science and Engineering*, 13 (2005)

