PAUL SCHERRER INSTITUT

PSI

Laboratory for Neutron and Muon INstrumentation

Gediminas Simutis :: Paul Scherrer Institute

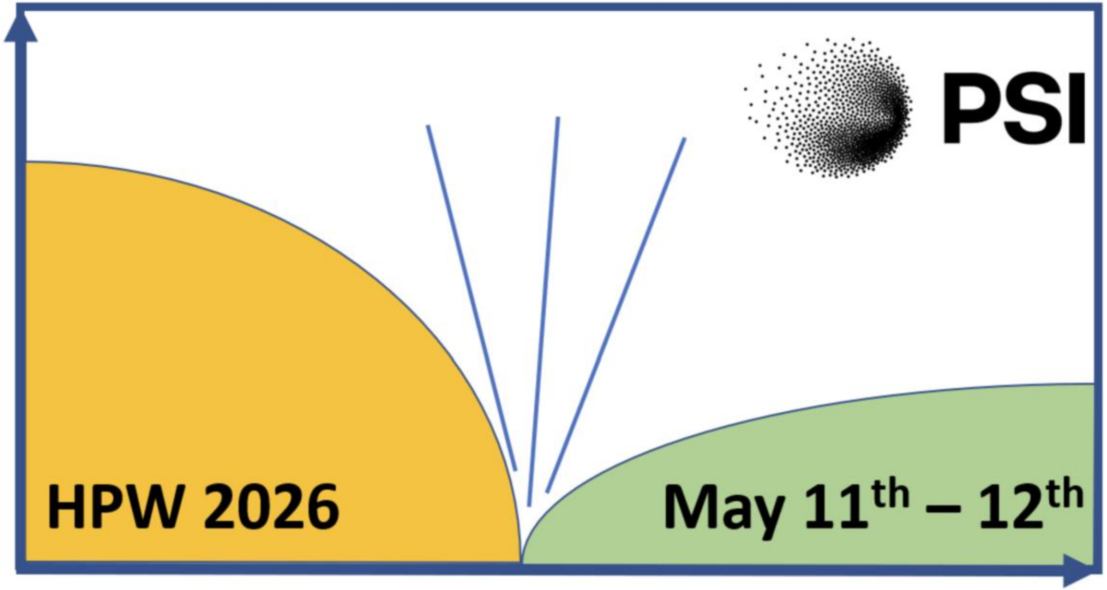
High Pressure Techniques for Neutrons, X-rays and muons

Sample Environment Training School

January 19th – 23rd 2026, Lund, Sweden

High-Pressure Workshop at PSI

PSI



High Pressure Workshop

May 11 – 12, 2026
PSI Villigen
Europe/Zurich timezone

https://indico.psi.ch/event/17608/

High-pressure **science** and **technical** developments for:
- neutrons
- X-rays
- muons
- and other techniques

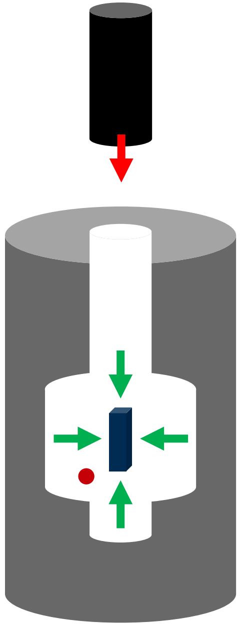
Plan for the lectures

- **Lecture 1:**

1. Why are we doing high pressure experiments?
2. What are the constituent parts?
3. How do we build the cells?
4. Different designs of the cells
5. How to measure pressure?
6. How do we transmit the pressure?

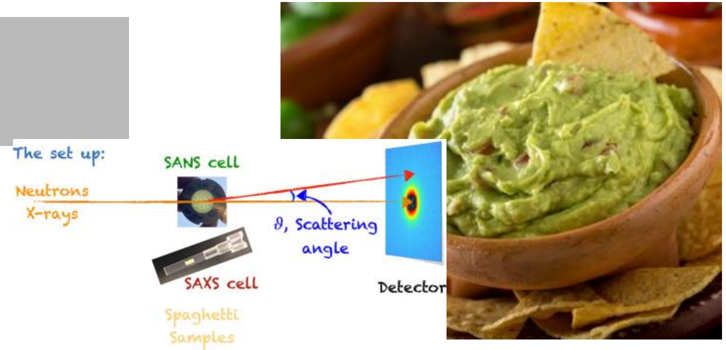
- **Lecture 2:**

1. Uniaxial pressure: different methods
2. Uniaxial pressure: tips and tricks
3. Pressure and background
4. Computing background
5. MuSR experiments at high pressure



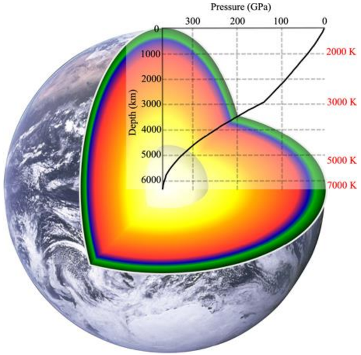
Why High Pressure?

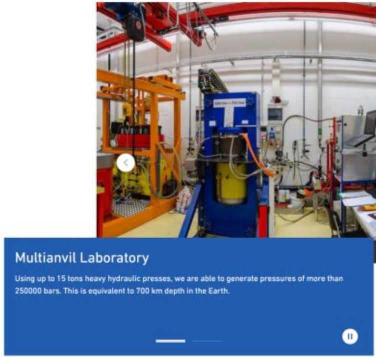
Food Sciences



Houston et al., Food Hydrocolloids 172, 111855 (2026)

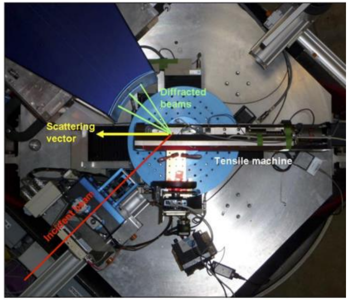
Earth Sciences





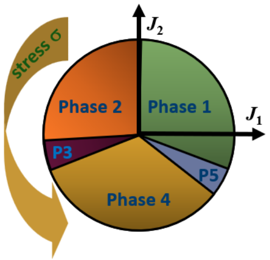
James W E Drewitt 2021 *J. Phys.: Condens. Matter* **33** 503004

Engineering materials



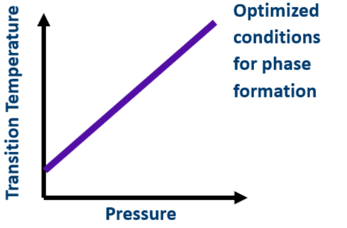
In-situ loading on POLDI, measuring the deformation mechanics of bainitic steels.

Fundamental Science



$$\mathcal{H} = J_1 \sum_{\langle ij \rangle_1} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle ij \rangle_2} \mathbf{S}_i \cdot \mathbf{S}_j$$

Guiding Design of New Materials

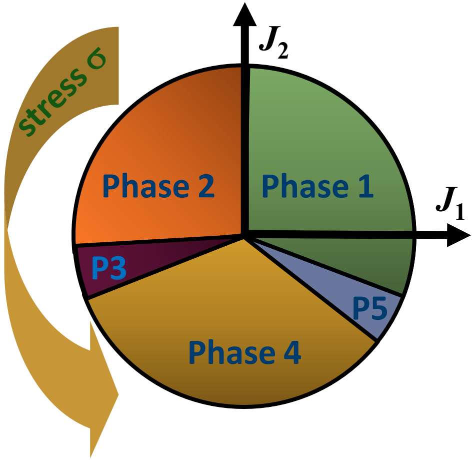


Why is high pressure research important?

PSI

(In condensed matter and for potential applications)

Engineering Hamiltonians



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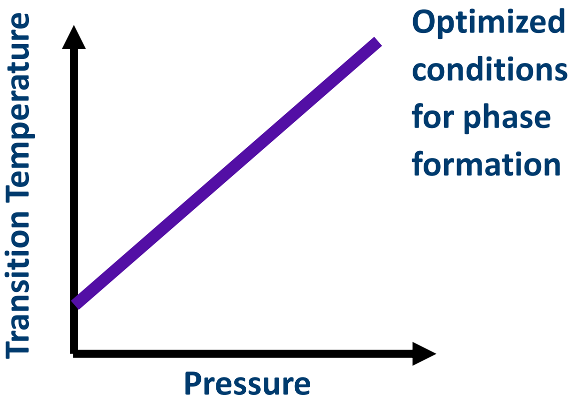

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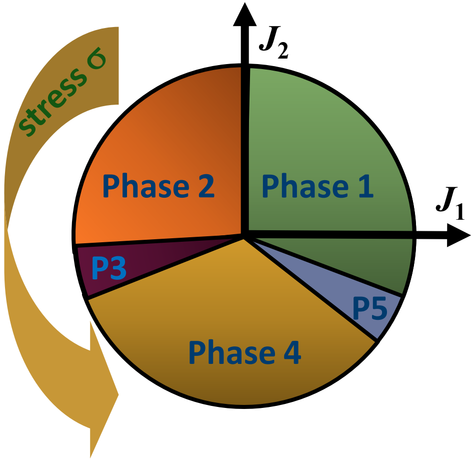

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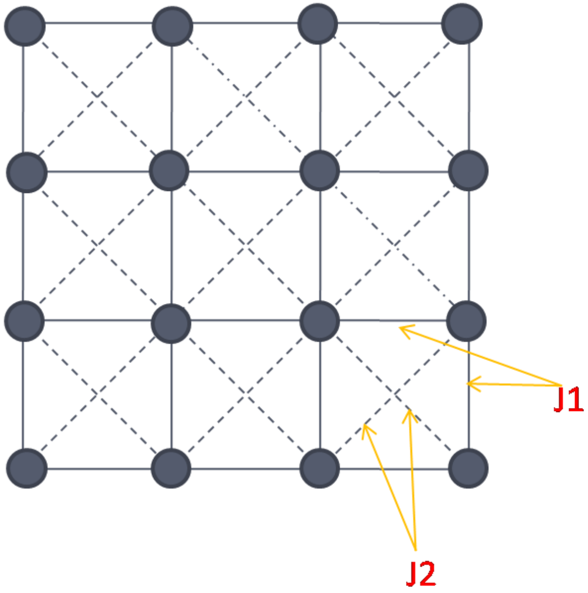
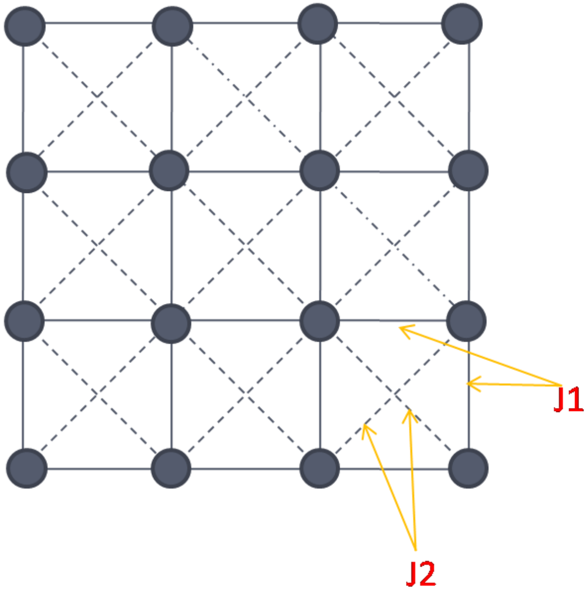
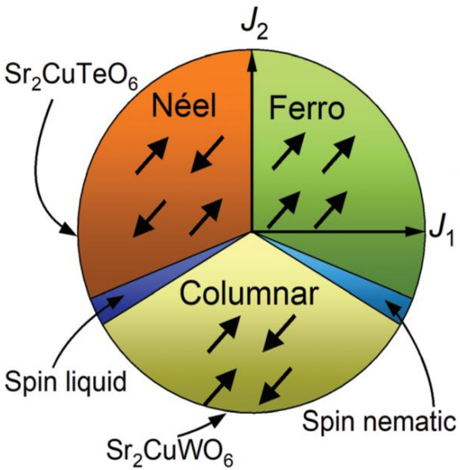


Shannon et al., 2006

Engineering Hamiltonians





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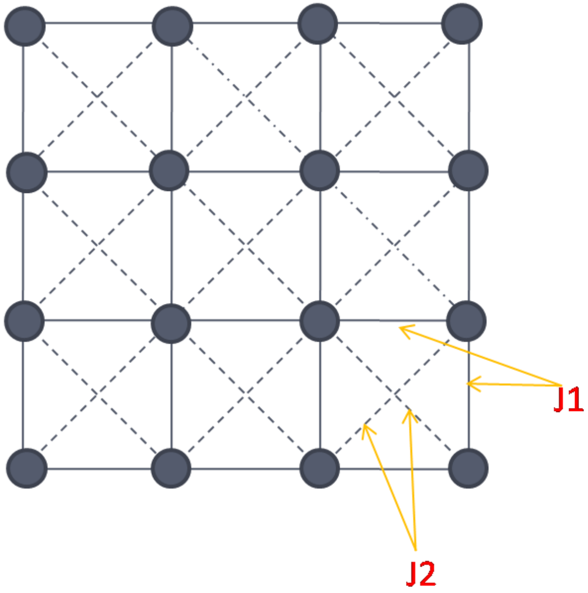

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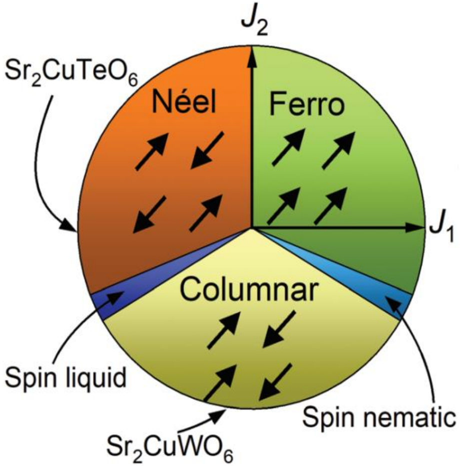

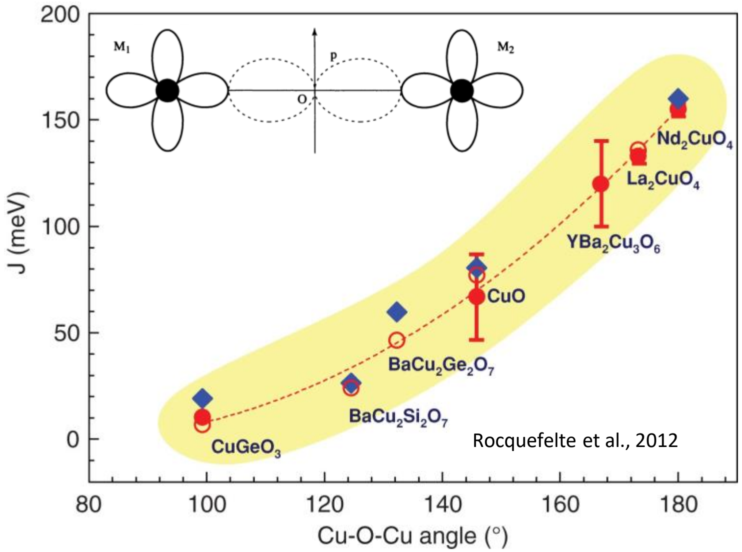

Rocquefelte et al., 2012

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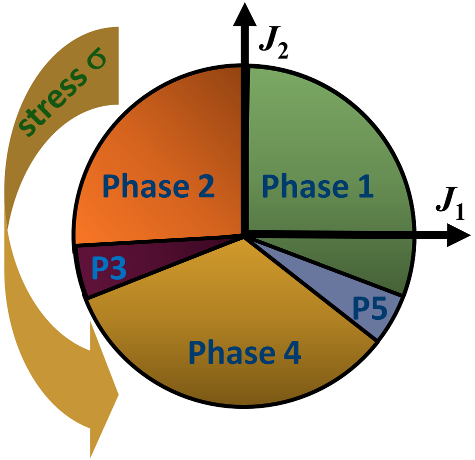
Why is high pressure research important?

(In condensed matter and for potential applications)

Engineering Hamiltonians



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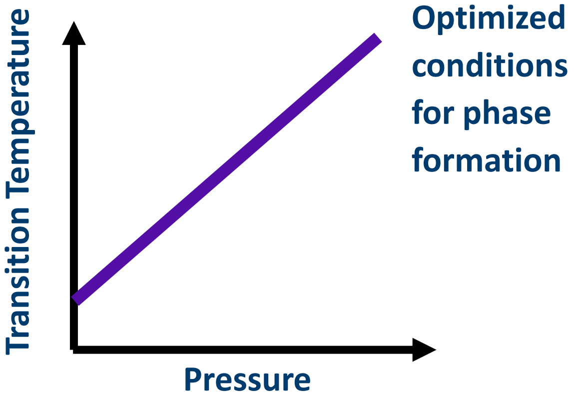
Guiding Design of New Materials



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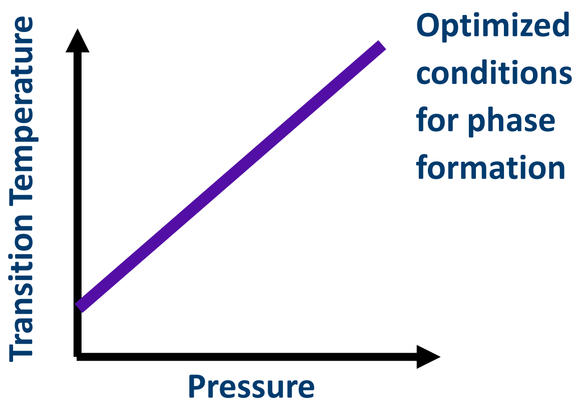
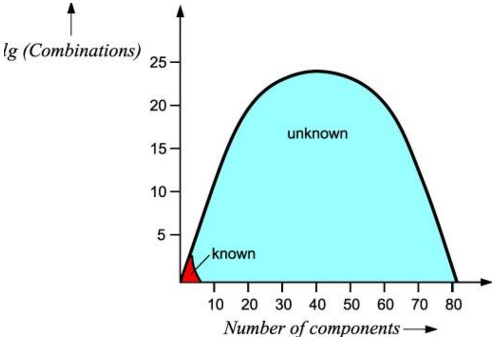


Materials discovery at high pressures

Lijun Zhang et al.,
Nature Reviews Materials 2, 17005 (2017)

Guiding Design of New Materials



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Jansen., Angew. Chem. **41**, 3746 (2002)

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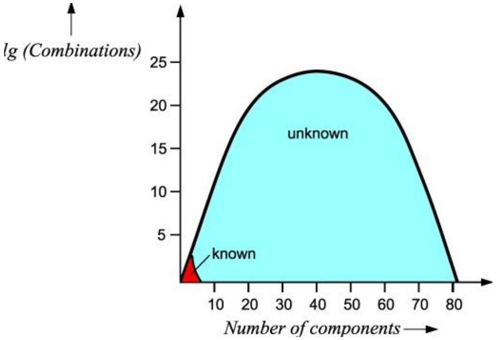

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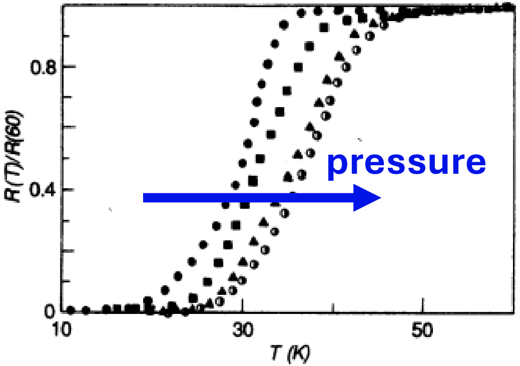
C. W. Chu,* P. H. Hor, R. L. Meng, L. Gao, Z. J. Huang

A superconducting transition with an onset temperature of 52.5 K has been observed under hydrostatic pressure in compounds with nominal compositions given by $(La_{0.9}Ba_{0.1})_2CuO_{4-y}$. Possible causes for the high-temperature superconductivity are discussed.



Guiding Design of New Materials

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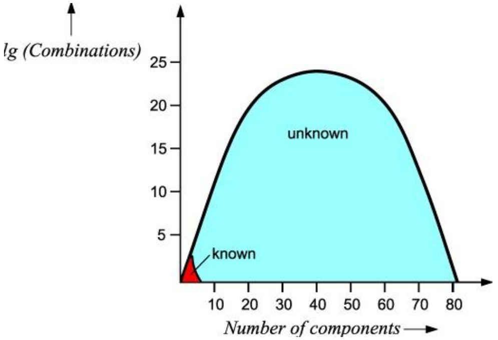

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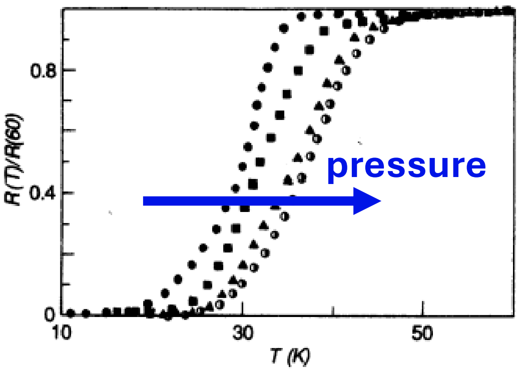


"chemical pressure"

Ba -> Y

Volume 58, Number 9 PHYSICAL REVIEW LETTERS 2 March 1987

Superconductivity at 93 K in a New Mixed-Phase Y-Ba-Cu-O Compound System at Ambient Pressure

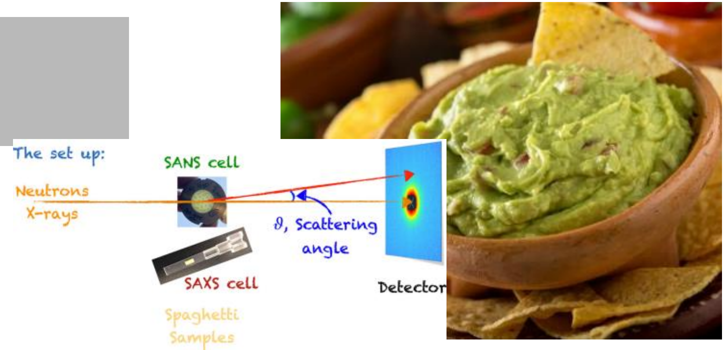
M. K. Wu, J. R. Ashburn, and C. J. Torng
Department of Physics, University of Alabama, Huntsville, Alabama 35899

and

P. H. Hor, R. L. Meng, L. Gao, Z. J. Huang, Y. Q. Wang, and C. W. Chu[a]
Department of Physics and Space Vacuum Epitaxy Center, University of Houston, Houston, Texas 77004
(Received 6 February 1987; Revised manuscript received 18 February 1987)

Why High Pressure?

Food Sciences



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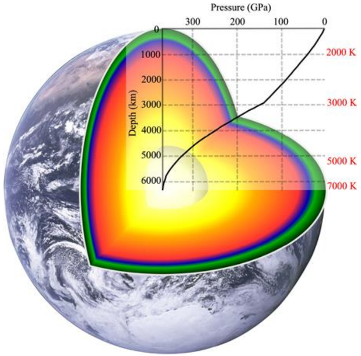
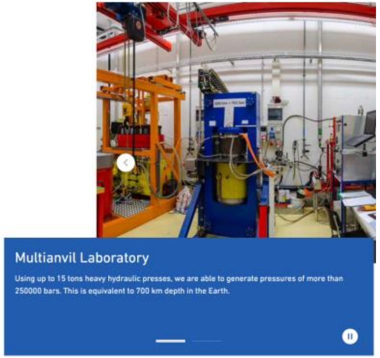
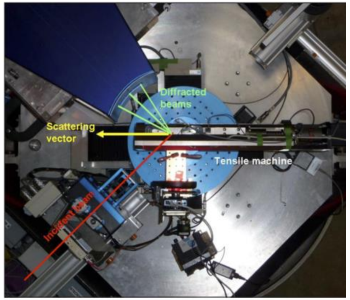




James W E Drewitt 2021 *J. Phys.: Condens. Matter* **33** 503004

Engineering materials



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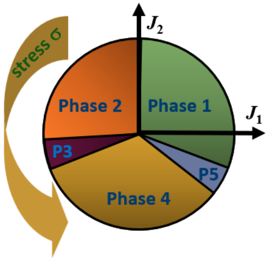
Fundamental Science



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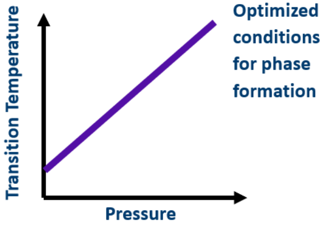
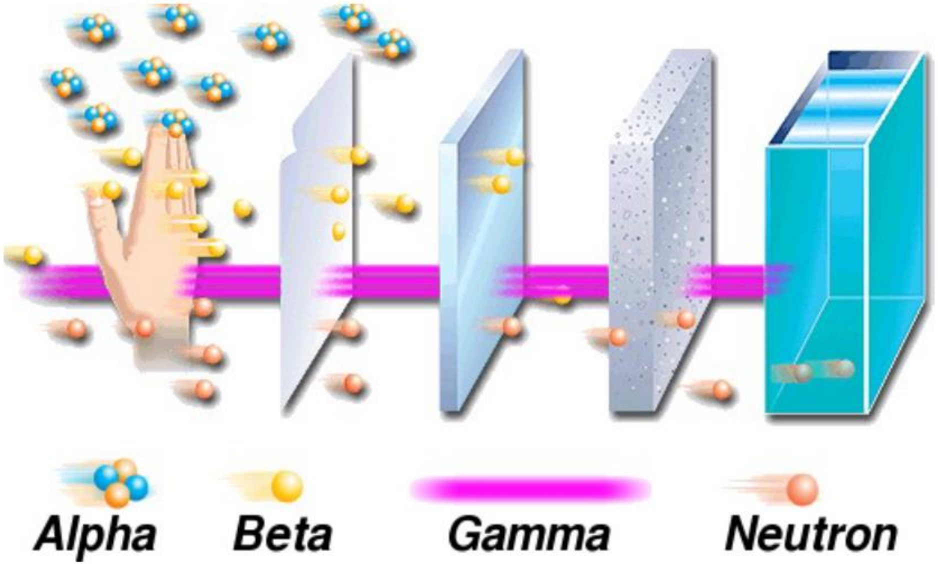
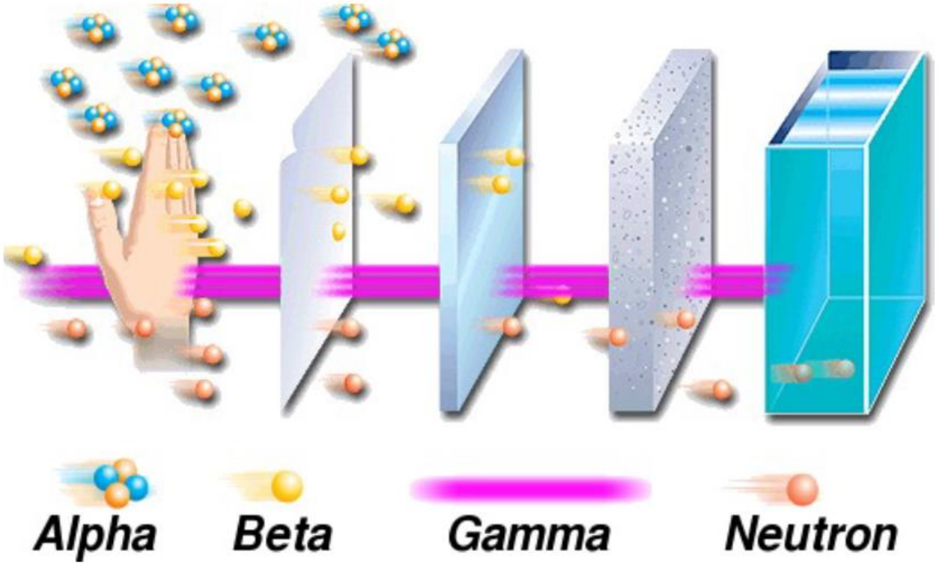


Properties of radiation

Properties of radiation



Properties of radiation



Implications of weak interaction for neutron experiments:

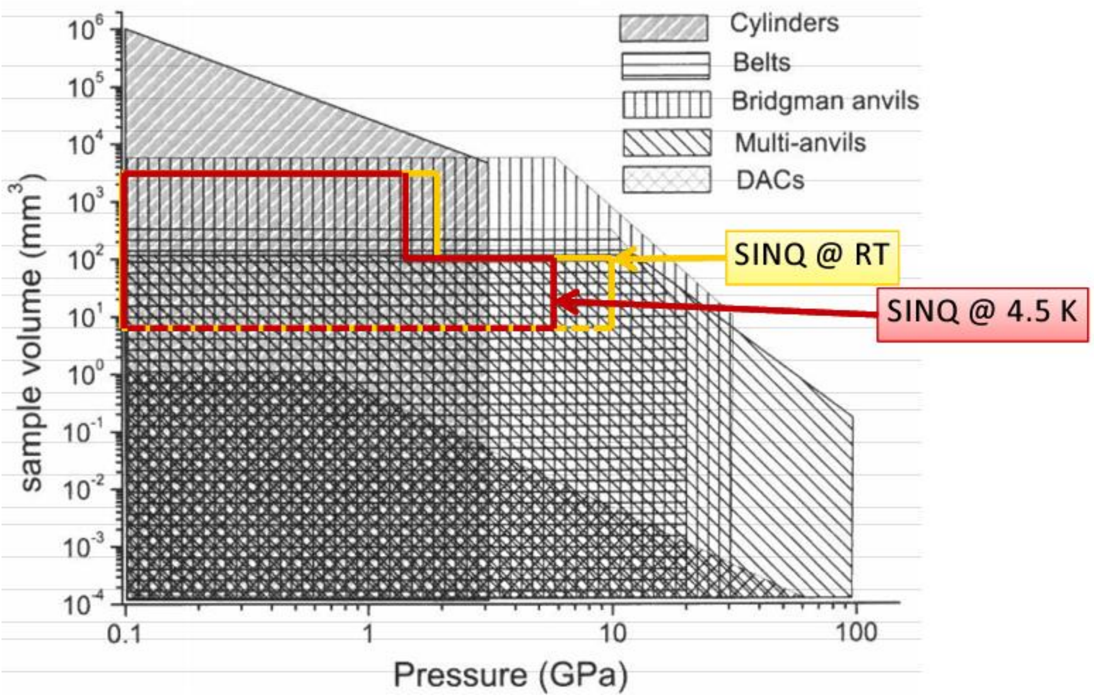
- Large samples are required

+ Works well with extensive SE

* The pain of setting up such experiments is worth it, because of the fantastic compatibility of energy (meV) and wavelength (0.1 nm) with properties at atomic level

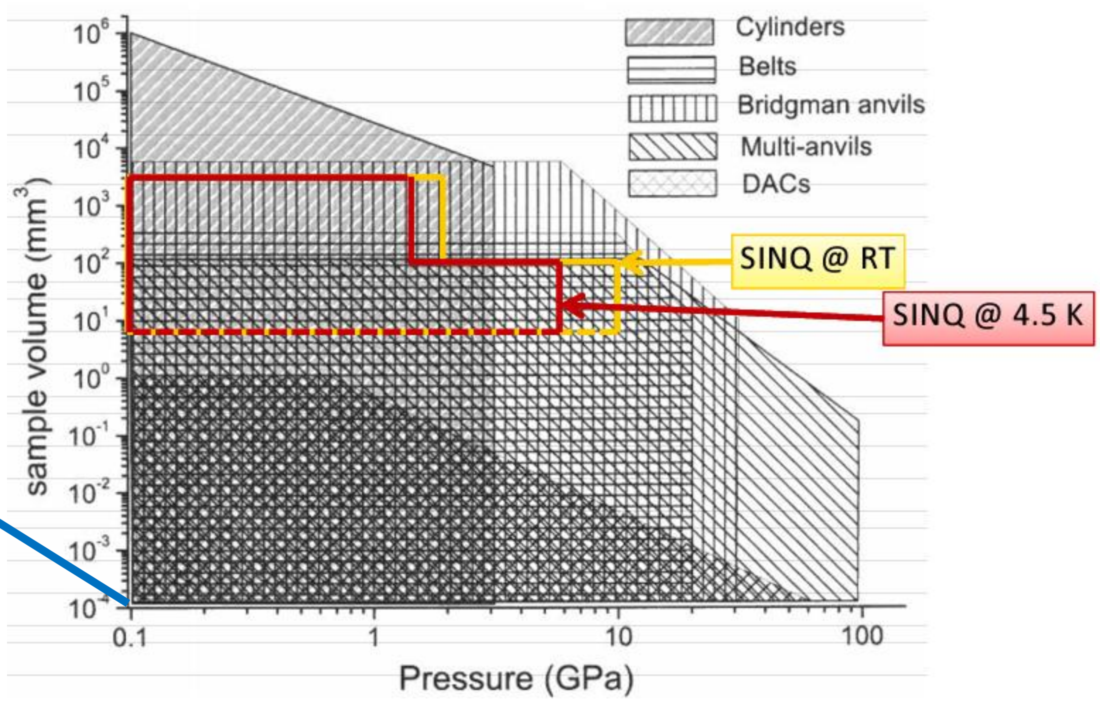
Fundamental Limitation: Volume OR Pressure

Fundamental Limitation: Volume OR Pressure



Techniques in High Pressure Neutron Scattering (Stefan Klotz)

Fundamental Limitation: Volume OR Pressure



Techniques in High Pressure Neutron Scattering (Stefan Klotz)

X-ray beam size << 1mm

DACs for everything

Neutron beam size >> 1mm

Variety of methods based on science needs

+ Other axes (B, T, chemicals)

Types of cells and constituent parts

Key ingredients for pressure generation

Pressure cell

- Clamp/piston pressure cells
- Anvil cells (DAC, BAC, PEC, multi-anvil cells)

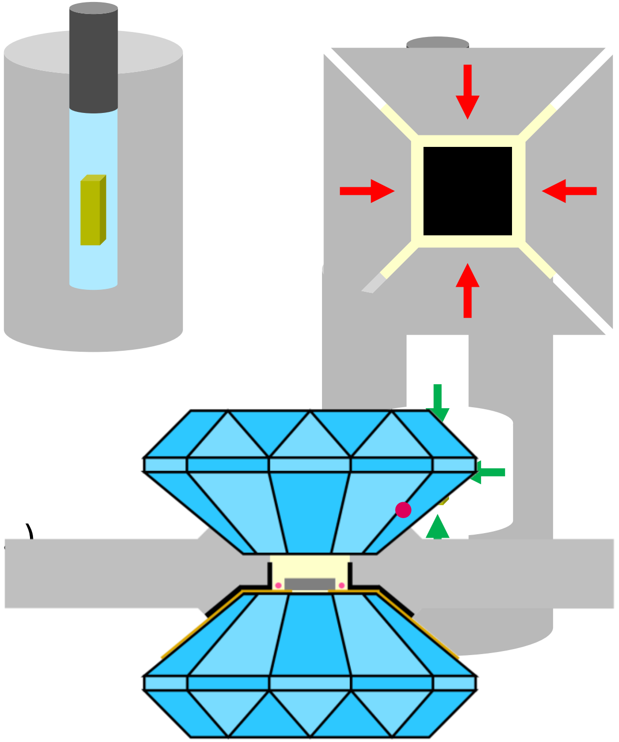
Pressure transmitting medium

- Liquid (Daphne oil, methanol:ethanol(:water), …)
- Solid (NaCl, pyrophyllite, …)
- Gas (He, N, Ar)

Pressure sensor

- Transport properties (manganin resistivity, T_c of In, Sn, Pb, …)
- Fluorescence (ruby), EOS (NaCl, Au, …), …

Patience and steady hands ☺



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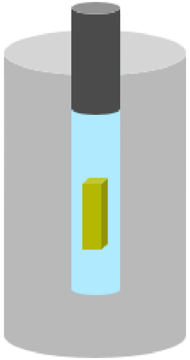
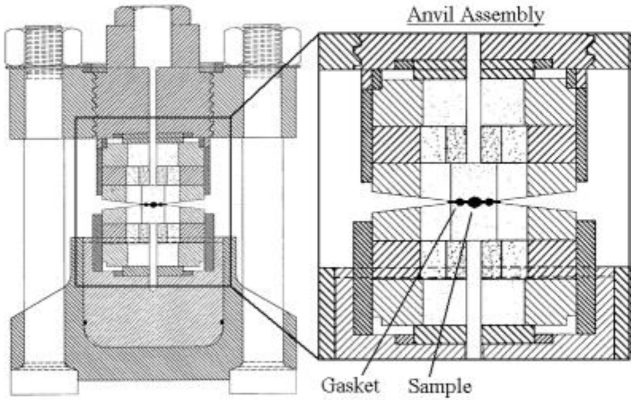
Different design of the cells

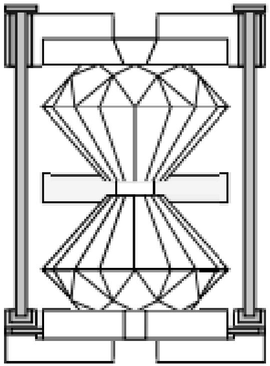
Piston cells



Paris-Edinburgh



DAC



Pressure

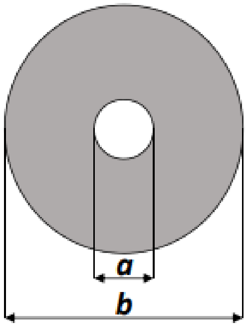
Volume

Piston - cylinder cells

- What is the maximum achievable pressure?

$$p^s_{\max} = \sigma_Y \left[\frac{1}{2} - \frac{a^2}{2b^2} \right],$$

Single-wall cylinder



- For b -> a, Pmax -> 0
- For a -> 0 and b -> inf., Pmax -> $\frac{1}{2}\sigma_Y$

- The single-cylinder strength is limited

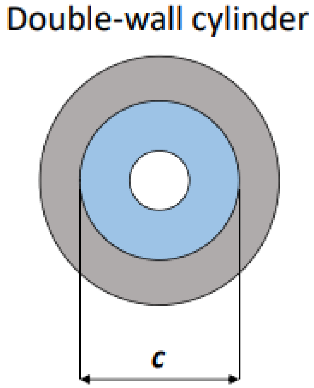
Khasanov et al., 2022

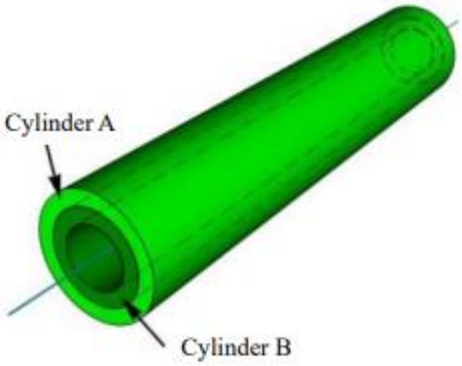
Piston - cylinder cells

- The interface has to provide the support:
  Hot-cold insertion
  Conical insertion

$$p^s_{\max} = \sigma_Y \left[\frac{1}{2} - \frac{a^2}{2b^2}\right],$$

$$p^d_{\max} = \sigma_Y \left[1 - \frac{a^2}{2c^2} - \frac{c^2}{2b^2}\right], \quad c = \sqrt{ab}$$





Khasanov et al., 2022

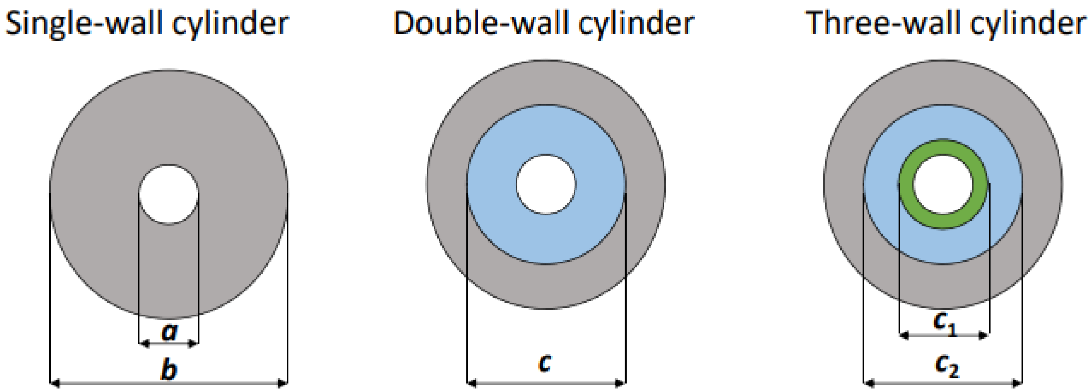
Piston - cylinder cells

- Basic considerations and limitations

$$p^s_{\rm max} = \sigma_{\rm Y}\left[\frac{1}{2} - \frac{a^2}{2b^2}\right],$$

$$p^d_{\rm max} = \sigma_{\rm Y}\left[1 - \frac{a^2}{2c^2} - \frac{c^2}{2b^2}\right],$$

$$p^t_{\rm max} = \sigma_{\rm Y}\left[\frac{3}{2} - \frac{a^2}{2c_1^2} - \frac{c_1^2}{2c_2^2} - \frac{c_2^2}{2b^2}\right].$$



$$c = \sqrt{ab}, \quad c_1 = \sqrt[3]{a^2 b}, \text{ and } c_2 = \sqrt[3]{ab^2}$$

Khasanov et al., 2022

Piston - cylinder cells

- Basic considerations and limitations

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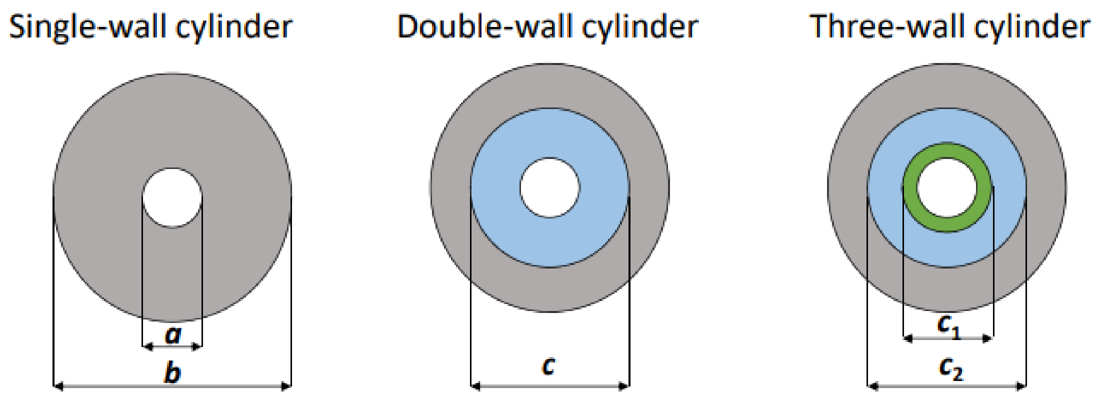


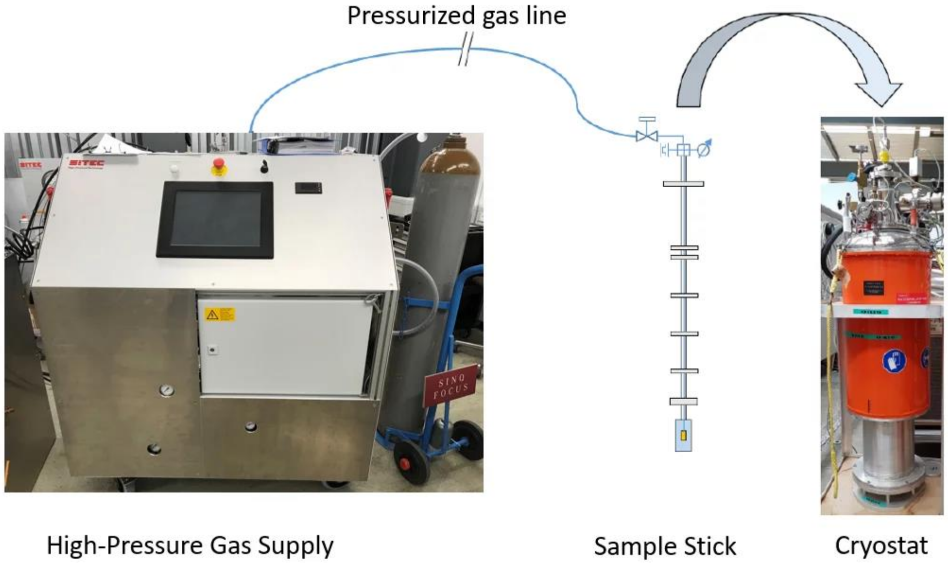
$$c = \sqrt{ab}, \quad c_1 = \sqrt[3]{a^2 b}, \text{ and } c_2 = \sqrt[3]{ab^2}$$

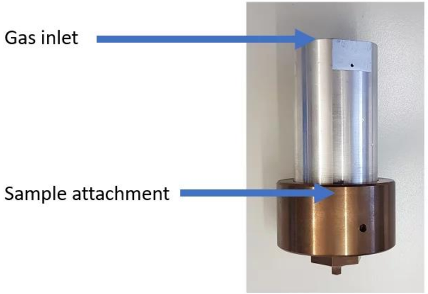
$$p^s_{\max} \div p^d_{\max} \div p^t_{\max} \simeq 1 \div 1.6 \div 1.92.$$

with $a = 6$ mm and $b = 24$ mm

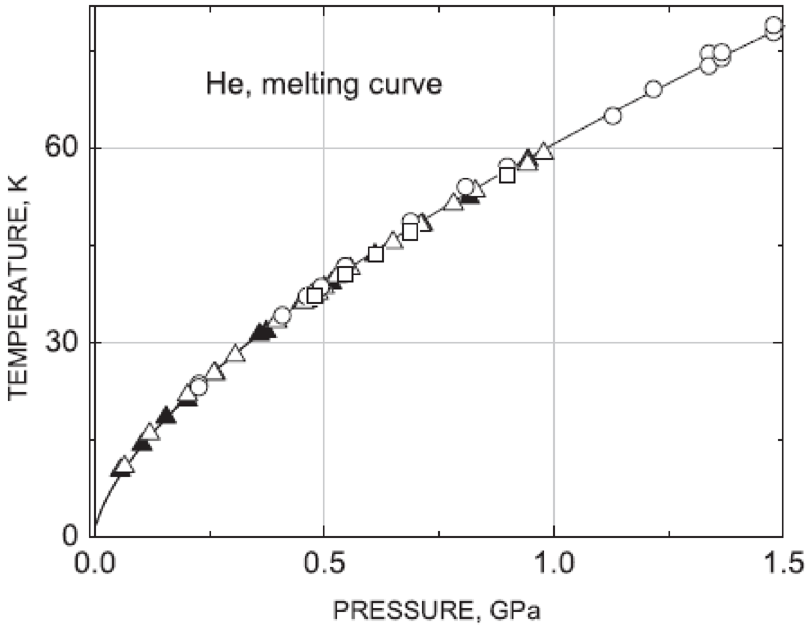
Khasanov et al., 2022

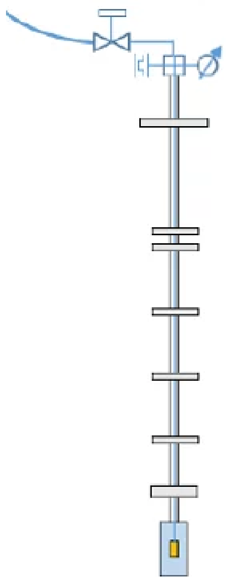
Al 5 kbar – single wall gas cell



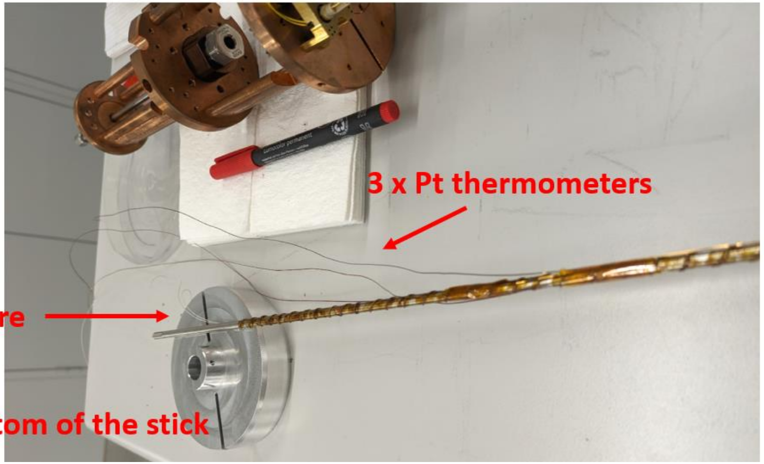


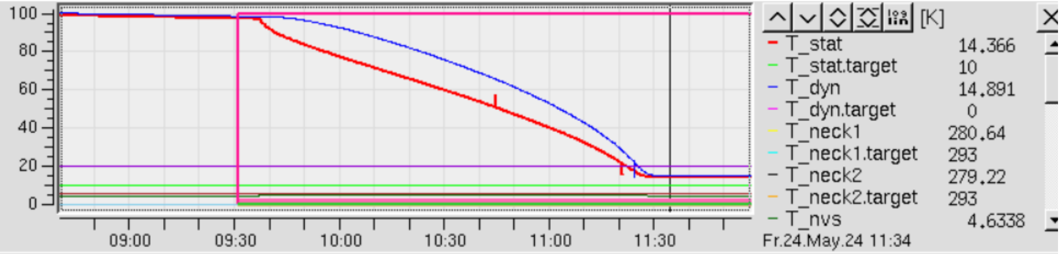
Gas cells -


He, melting curve
TEMPERATURE, K
PRESSURE, GPa
0
30
60
0.0
0.5
1.0
1.5


RT He gas
LT Solid He

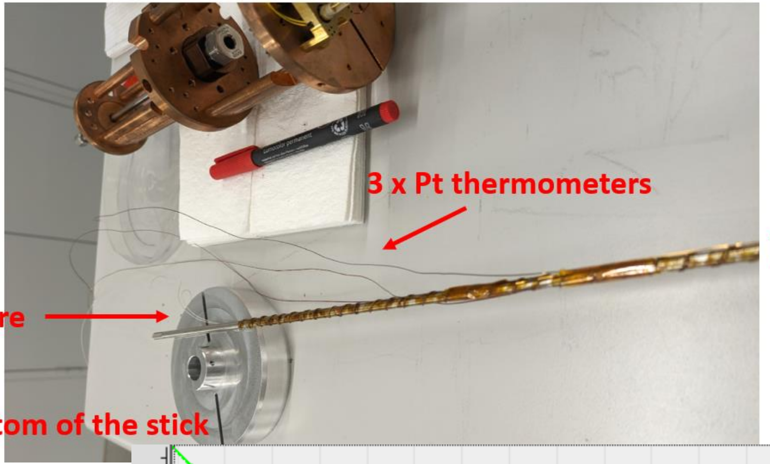
Gas cells -

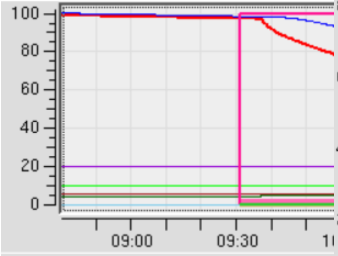


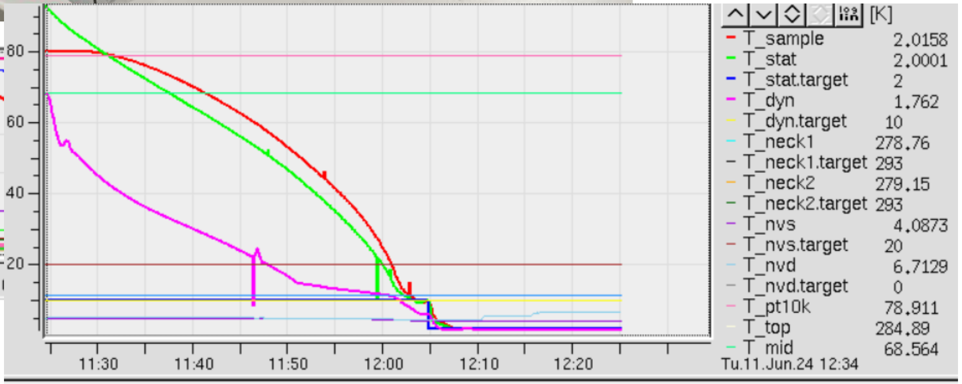


If the heater is on, the lowest T is limited

Gas cells -

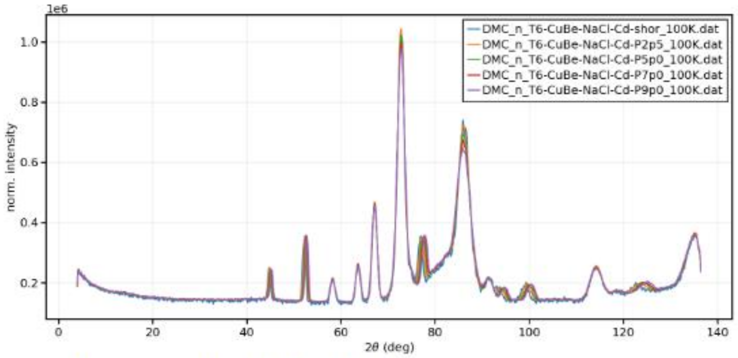


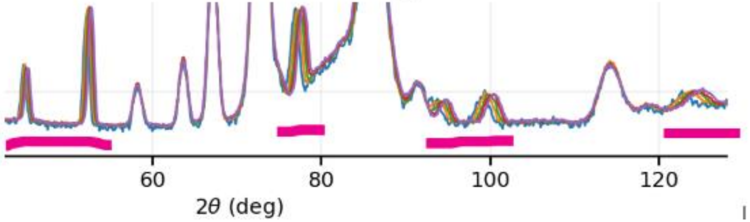




With the heater off, T < 2 K

TAV6-CuBe two-wall cell

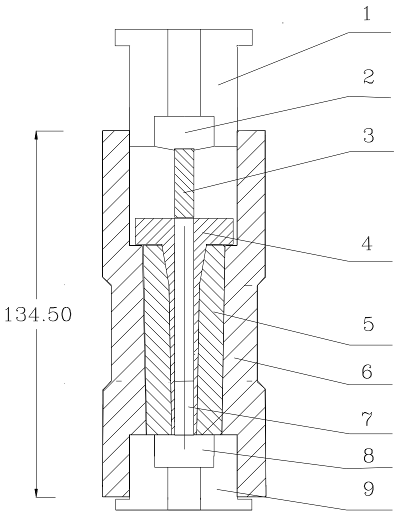




Standard clamp cells

Standard clamp cells - I

12 kbar cell for inelastic neutron scattering / single crystal wide-angle diffraction



1,9.-Nuts, steel

2,8.-Pistons support, steel

3,7.-Pistons, steel and WC

4.-Insert1, hard steel

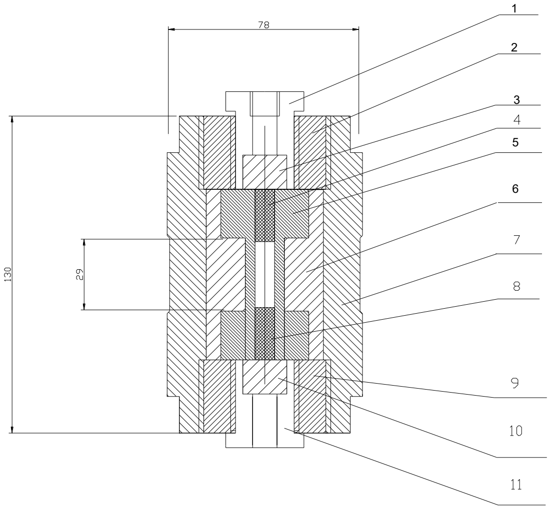
5.-Insert2, hard Al alloy

6.-Cells body, hard Al alloy.

- *T* down to 1.5 K (then 10 kbar max *P*)
- Outer diameter = 55 mm
- Inner diameter (for sample) = 7.4 mm
- Weight = 1.6 kg

Standard clamp cells - II

17 kbar cell for inelastic neutron scattering / single crystal wide-angle diffraction



1,11.-Nuts1, steel

2,9.-Nuts2, steel

3,10.-Pistons support, steel

4,8.-Pistons, steel and WC

5.-Insert1, hard steel

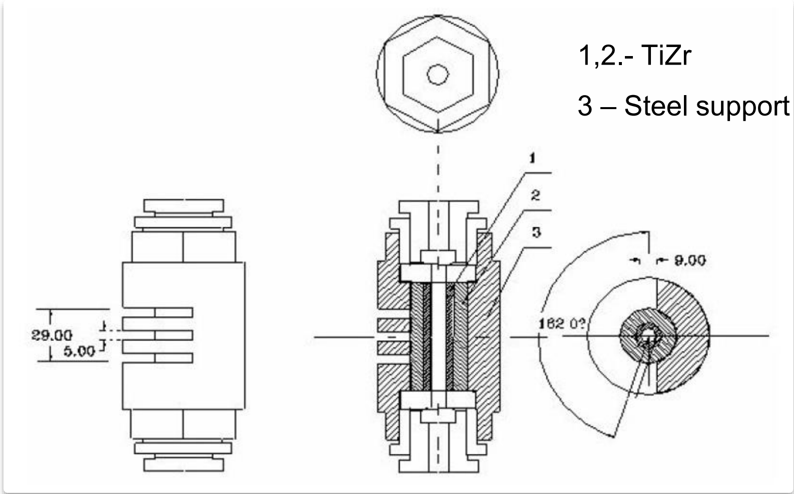
6.-Insert2, hard Al alloy

7.-Cells body, hard Al alloy.

- *T* down to 1.5 K (then 15 kbar max *P*)
- Outer diameter = 78 mm
- Inner diameter (for sample) = 7.8 mm
- Weight = 2.6kg

Standard clamp cells - III

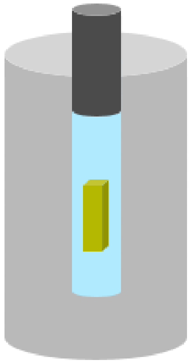
Workhorse **15 kbar** cell for neutron powder diffraction



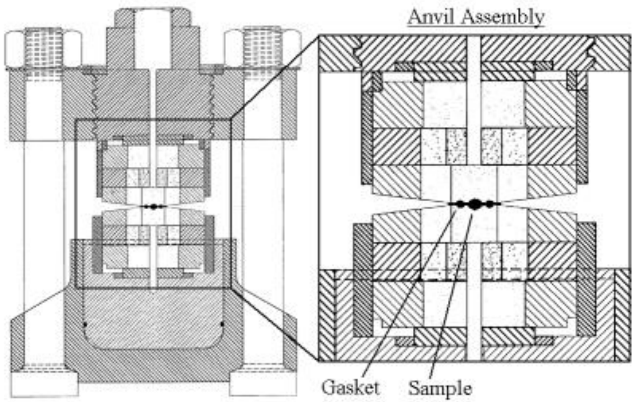
- *T* down to 1.5 K (then 12-14 kbar max *P*).
- Outer diameter = 78 mm
- Inner diameter (for sample) = 8 mm
- TiZr ‘null-scattering’ alloy

Different design of the cells

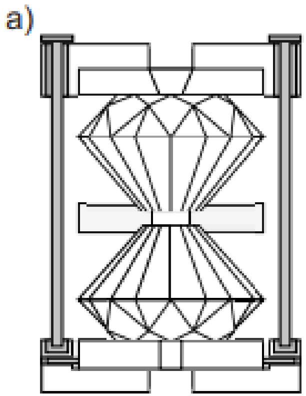
Piston cells



Paris-Edinburgh



DAC



Pressure →

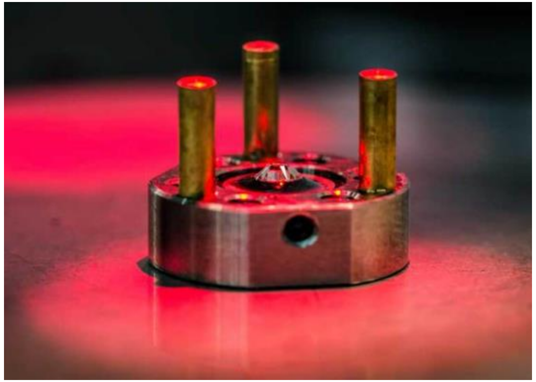
← Volume

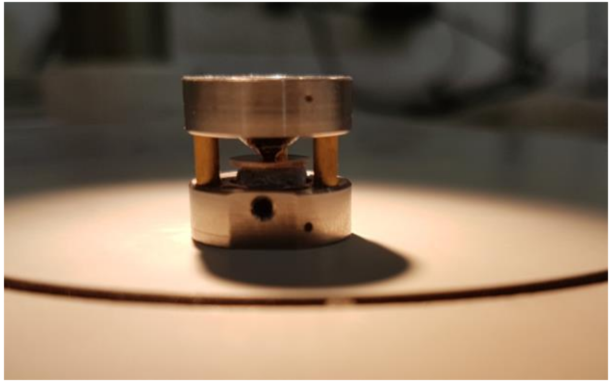
Diamond Anvil Cells

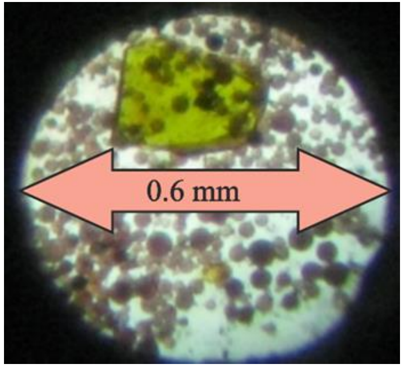
Highest pressures available – 100s of GPa

As usual - volume or pressure

Gasket technology and preparation is key

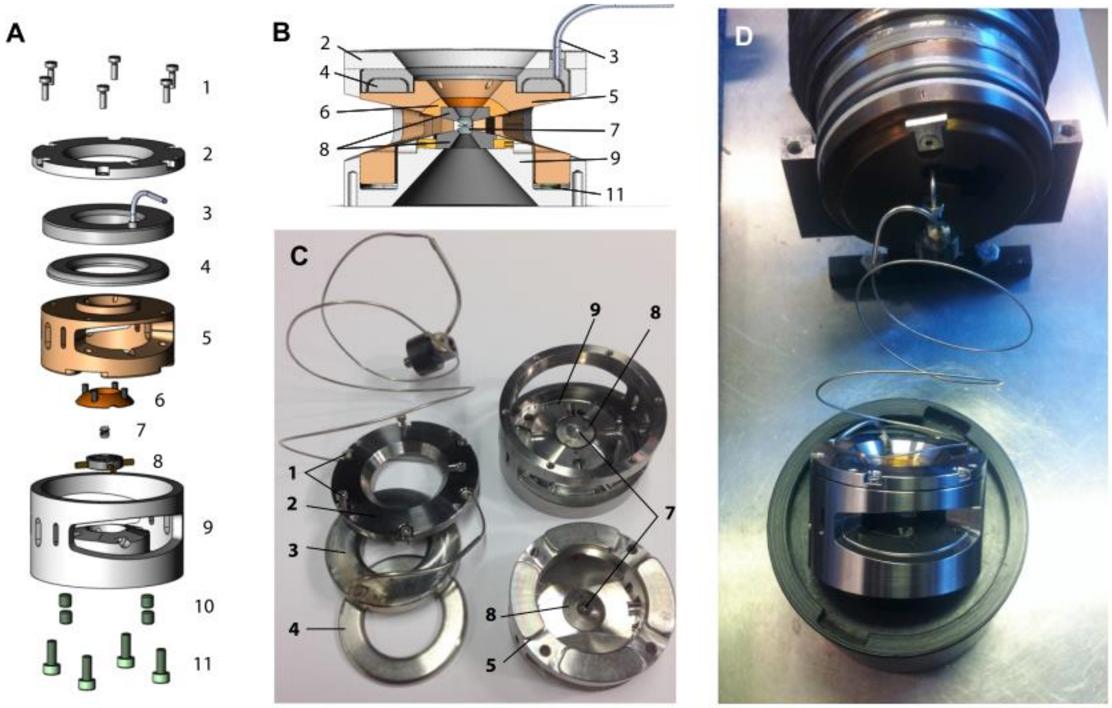






Diamond Anvil Cells

Diamond Anvil Cells – from Universal



A versatile diamond anvil cell for X-ray inelastic, diffraction and imaging studies at synchrotron facilities

Cite as: Rev. Sci. Instrum. 90, 095107 (2019); doi: 10.1063/1.5119025
Submitted: 8 July 2019 • Accepted: 25 August 2019 •
Published Online: 25 September 2019

Sylvain Petitgirard,[1,a)] Jeroen Jacobs,[2] Valerio Cerantola,[2] Ines E. Collings,[2] Remi Tucoulou,[2] Leonid Dubrovinsky,[1] and Christoph J. Sahle[2,a)]

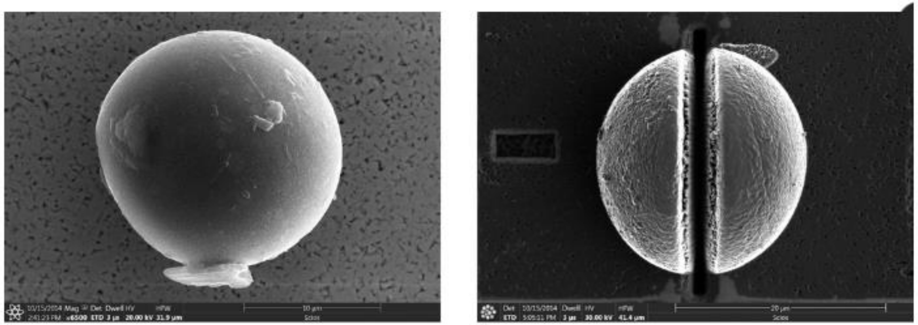
FIG. 1. The mBX110 design. (a) Exploded view of the mBX110 that shows the different parts with: (2) the membrane ring holder fixed with 6 M2 screws (1), (3) the gas membrane, (4) the membrane spacer, (5) the piston, (6) a rocker seat, (7) conical diamonds, (8) a flat tungsten carbide seat, (9) the cylinder, (10) stop screws, and (11) pressurizing screws. (b) Cross-sectional view of the mBX110, numberings are the same as for A. (c) Picture of the different parts of the mBX110. (d) A picture of the mBX110 after gas loading using the membrane at the ESRF.

Diamond Anvil Cells – to Record Breaking

Terapascal static pressure generation with ultrahigh yield strength nanodiamond

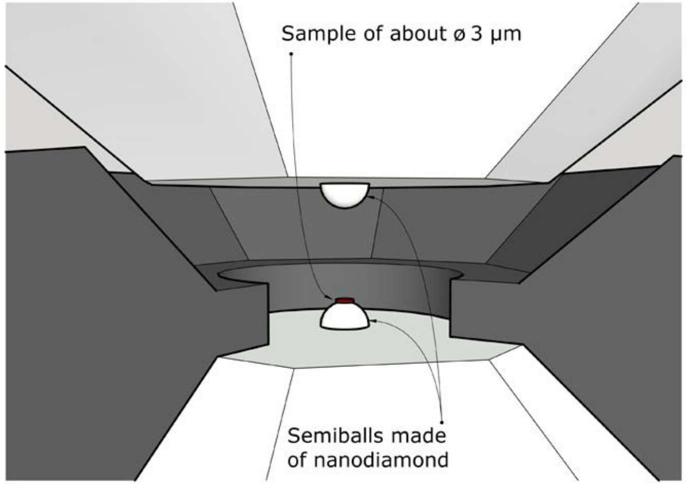
NATALIA DUBROVINSKAIA, LEONID DUBROVINSKY, NATALIA A. SOLOPOVA, ARTEM ABAKUMOV, STUART TURNER, MICHAEL HANFLAND, ELENA BYKOVA, MAXIM BYKOV, CLEMENS PRESCHER, VITALI B. PRAKAPENKA, SYLVAIN PETITGIRARD, IRINA CHUVASHOVA, BILIANA GASHAROVA, YVES-LAURENT MATHIS, PETR ERSHOV, IRINA SNIGIREVA, AND ANATOLY SNIGIREV fewer Authors Info & Affiliations

SCIENCE ADVANCES • 20 Jul 2016 • Vol 2, Issue 7 • DOI: 10.1126/sciadv.1600341



A B

Fig. 6 Images of an NCD ball before and after the FIB milling.
(**A**) Secondary electron image of a ball before ion milling, as taken in the Scios DualBeam system (FEI Deutschland GmbH) at a voltage of 20 kV and a current of 0.8 nA. mag, magnification; Det, detector; ETD, Everhart Thornley detector; HV, high voltage; HFW, horizontal field width. (**B**) Gallium ion image of the same ball (taken at 30 kV and 30 pA) after milling at 30 kV and 5 nA.



B

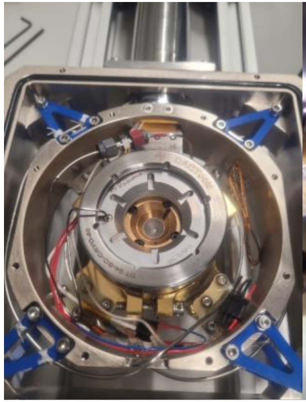
Fig. 7 Schematic drawings of the setup for ultrahigh static pressure generation.
(**A**) Testing of the performance of a single semiball forced against the diamond anvil in a LiF pressure medium in a conventional DAC. (**B**) ds-DAC assembly (not to scale) for experiments at ultrahigh pressures (above 1 TPa). Two transparent NCD semiballs were used as secondary anvils in a conventional DAC. Diameter of the NCD semiballs is ~20 μm, and the initial size of the sample is about 3 μm in diameter and about 1 μm in thickness.

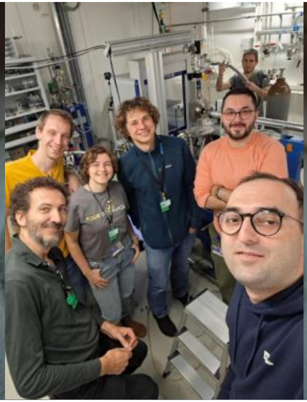
XRD DAC at PSI – moderate, but very useful

DAC Tools mSSDAC-80

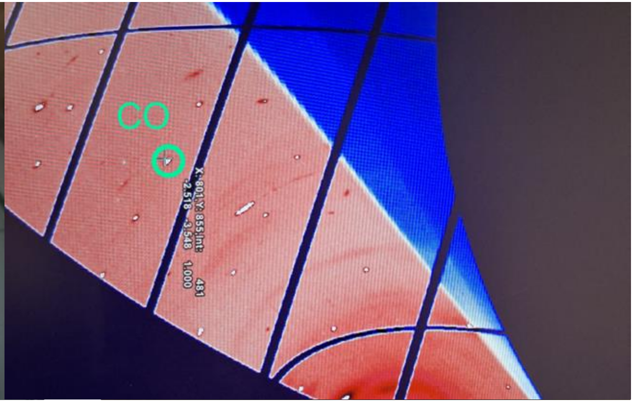
- ADDAMS (N. P. M. Casati) & I15 (B. Ghosh) beamlines
- Culet 0.5 mm, accessible $p \approx 20$ GPa
- Pressurizing – membrane (He gas)
- DAC Tools He-flow cryostat (lowest $T \approx 10$ K)

DAC Tools
Custom Equipment for High-Pressure Research
www.DACTools.com

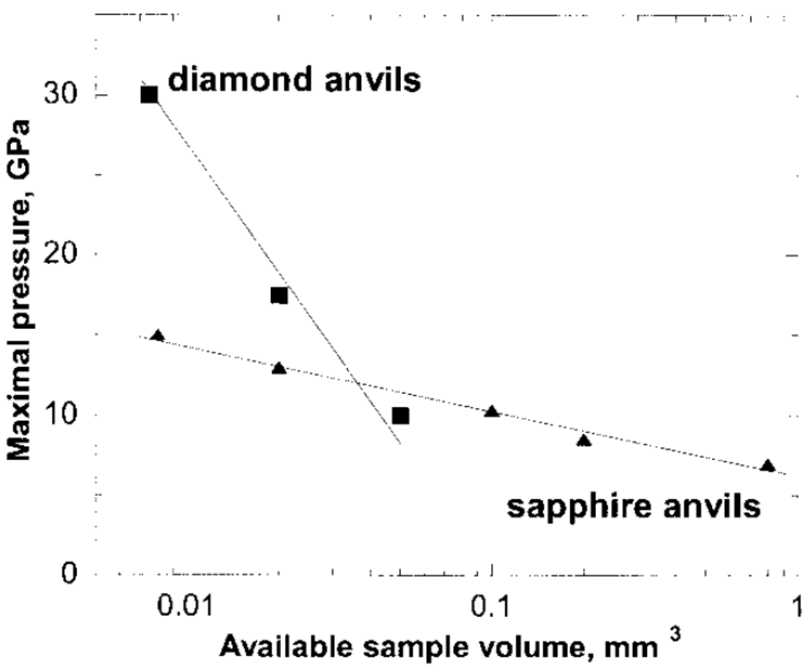




YRu_3Si_2 (4.5 GPa, 100 K)



Kurchatov-LLB cells



High Pressure Research
Vol. 24, No. 1, March 2004, pp. 193–204

Taylor & Francis
Taylor & Francis Group

NEUTRON DIFFRACTION EXPERIMENTS IN DIAMOND AND SAPPHIRE ANVIL CELLS

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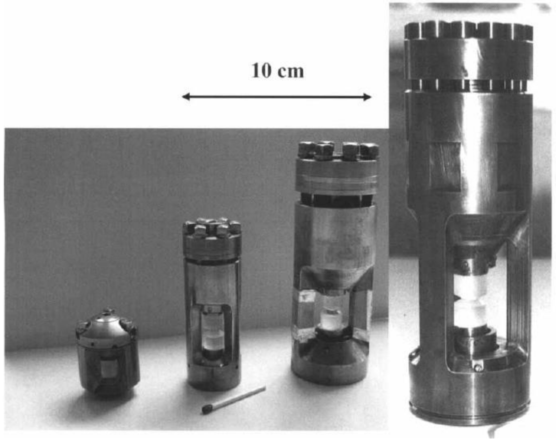
(Received 15 July 2003; Revised 6 November 2003; In final form 10 November 2003)

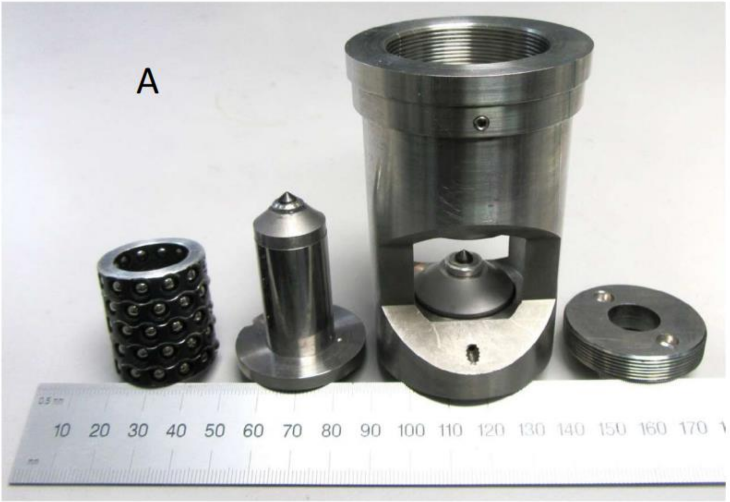


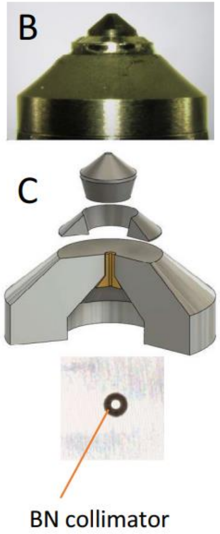
A new take at ORNL

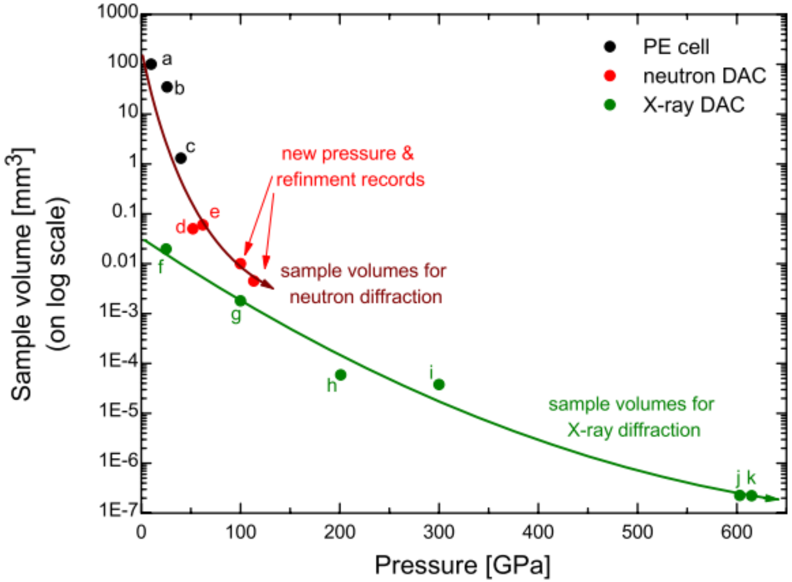
Advancing neutron diffraction for accurate structural measurement of light elements at megabar pressures

Bianca Haberl, Malcolm Guthrie & Reinhard Boehler

Scientific Reports **13**, Article number: 4741 (2023) | Cite this article







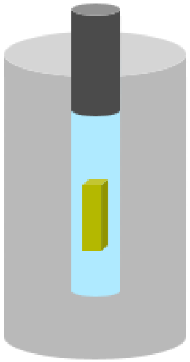
Cullet diameter approaching 1mm

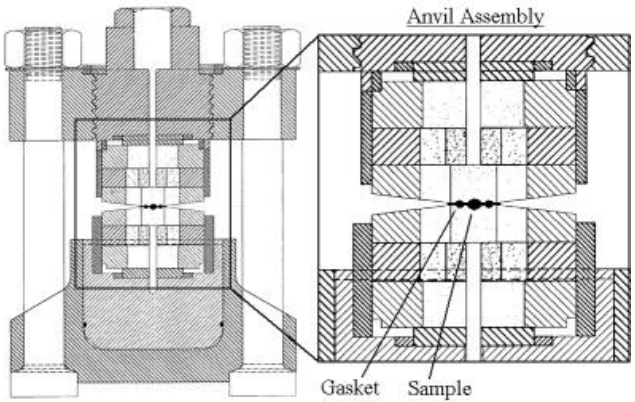
Different design of the cells

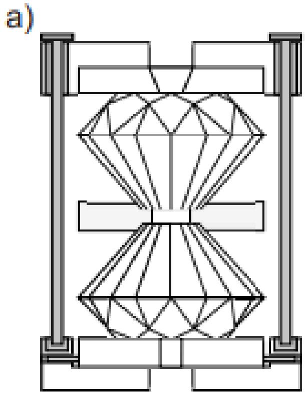
Piston cells

Paris-Edinburgh

DAC







Pressure

Volume

PAUL SCHERRER INSTITUT

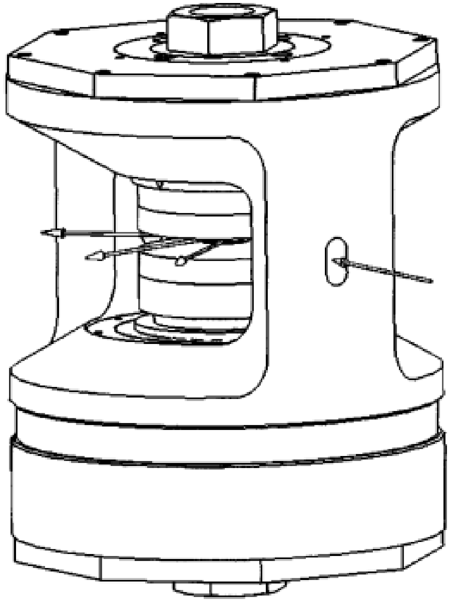
Paris-Edinburgh Press

<u>Opposed anvil technique</u>

Neutron absorbing cBN anvils (or other alternatives – ZTA, SD)

TiZr or CuBe gaskets

Sample Volume 30-100 mm^3



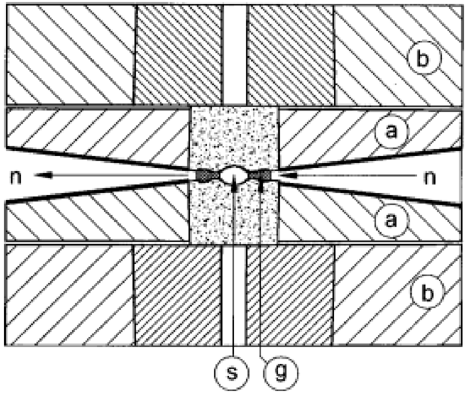


FIG. 1. Upper: VX Paris–Edinburgh press indicating the scattering geometry with the incident and diffracted neutron beams. The diameter of the press is 250 mm, its mass 60 kg. Lower: enlarged cross section of the anvil assembly: (a) anvils (speckle: cubic boron nitride, wide hatch: steel binding ring); (b) backing seats (narrow hatch: tungsten carbide, wide hatch: steel binding ring); (s) sample chamber; (g) gasket made of zero-scattering TiZr alloy. Bold lines on the anvil faces indicate 0.2 mm cadmium shielding. The diameter of the assembly is 90 mm.

Paris-Edinburgh Press – ever evolving

Regularly used at varied temperatures

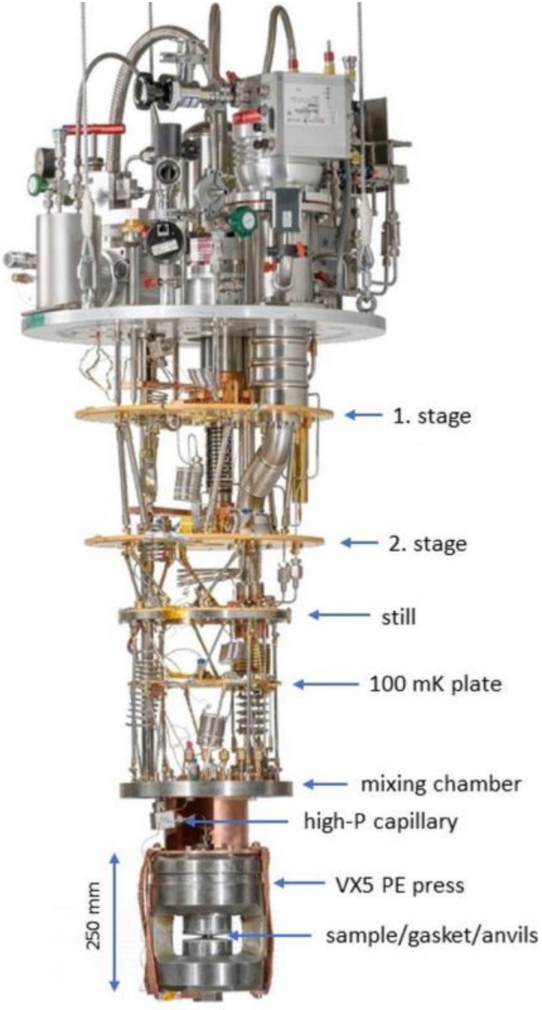
Recent innovation – DR + PE

Klotz et al., APL **127**, 211904 (2025)

Measurements at 160 mK and 20 GPa

On the opposite side: 3-4 GPa with higher volumes (ISIS)

Compatibility with high fields



Determining the pressure

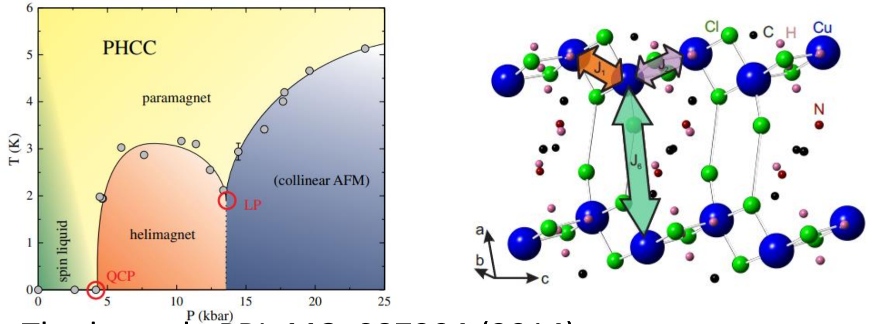
Determining the pressure

A cautionary story “no second transition”

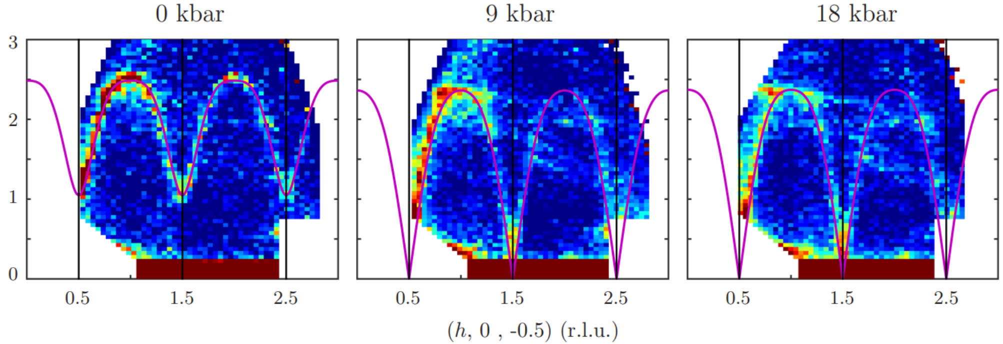
Nominal pressure was
taken based on calibration tables

Led to wrong interpretations,
which were corrected after subsequent
experiments

You really should know the pressure!



Thede et al., PRL **112**, 087204 (2014)



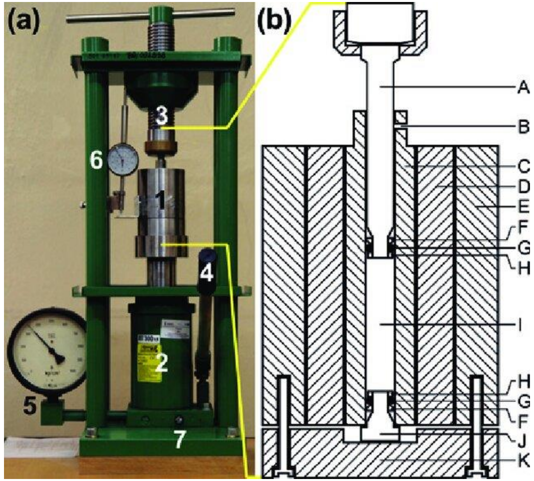
Perren, et. al PRB 92, 054413 (2015)

Bettler, et. al PRB 96, 174431 (2017)

Determining the pressure

Read out the gas pressure

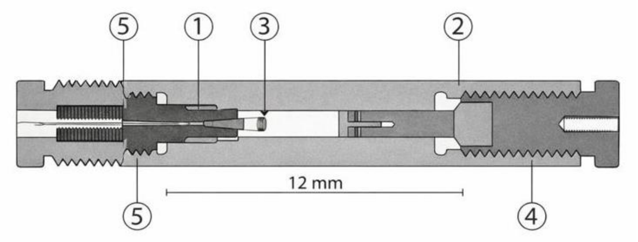
For clamp cells –
estimated based on the P applied



High-Pressure Gas Supply

Determining the pressure

Resistance of manganin
(HMI cell)



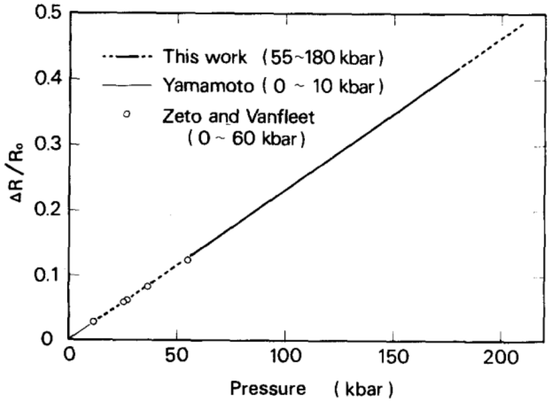
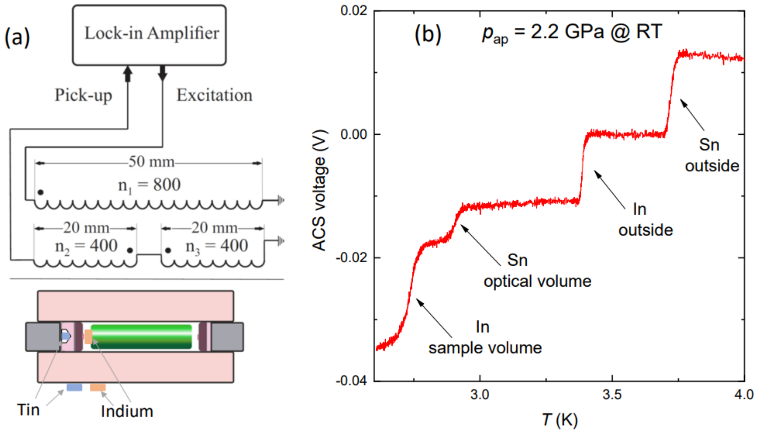


FIG. 3. Comparison of the present result and two results under hydrostatic condition for Manganin resistance versus pressure.

Fujioka 1978

Superconducting transition P-dependence
AC susceptibility

Khasanov 2016, Naumov 2022



Determining the pressure

Fluorescence, for example, Ruby lines

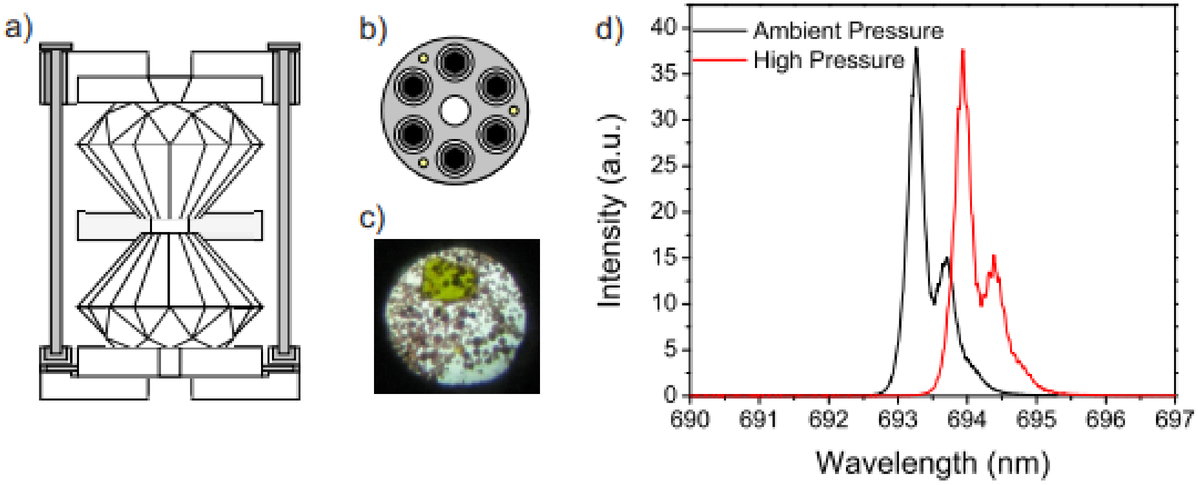
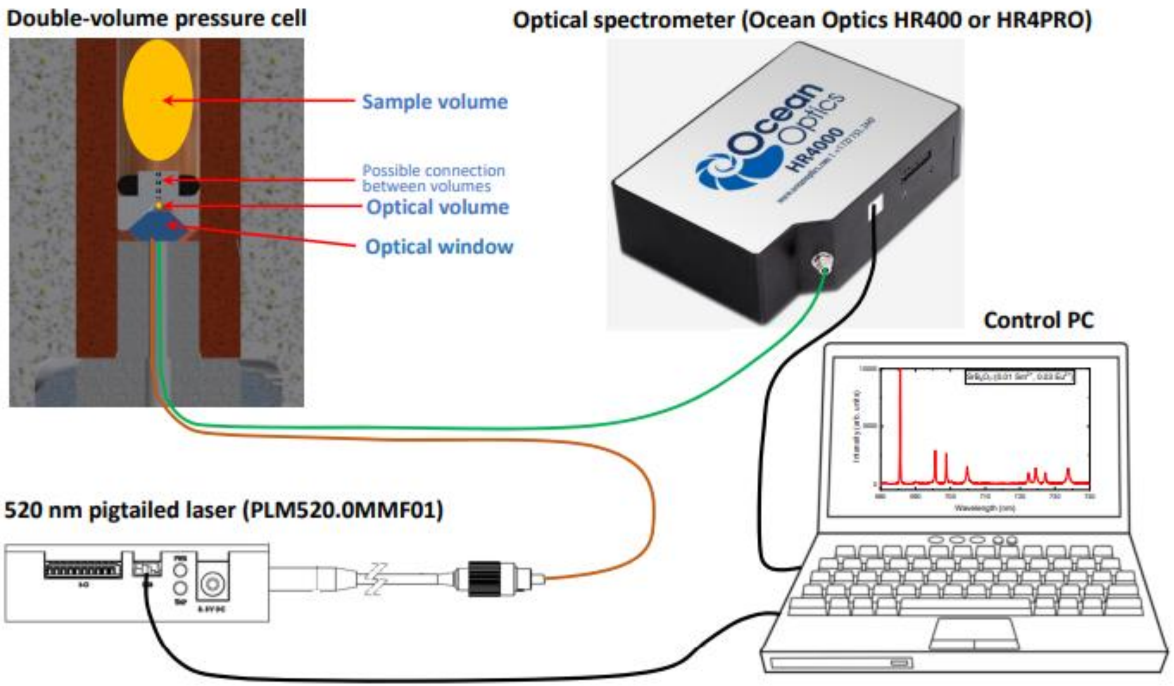
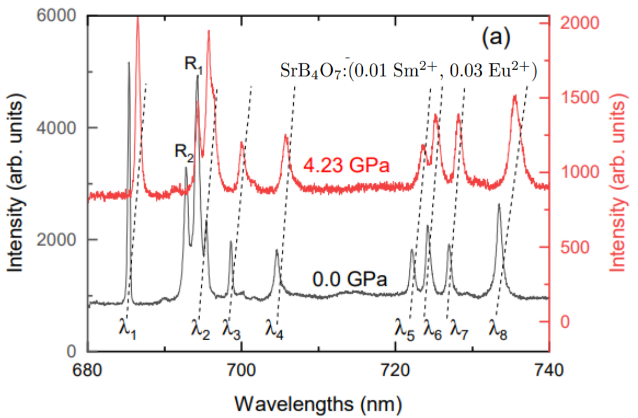


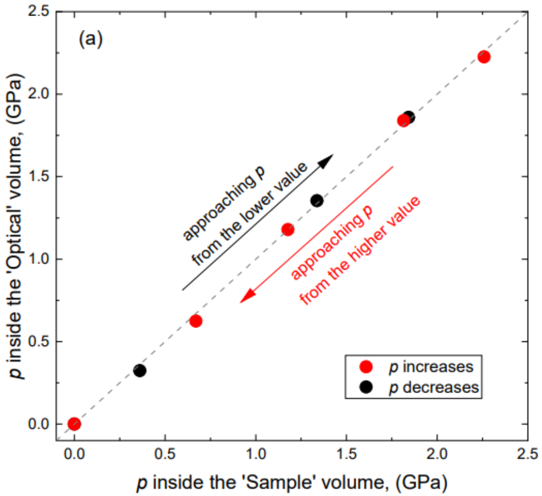
Figure 4.10: Diamond anvil pressure cell used in this thesis to achieve high pressure in Raman experiments. Panel a) shows the side view and b) shows the top view. The inside of the cell is shown in c) where the sample (green slab) and rubies (red spheres) are visible. The diameter of the sample space is 600 μm. The pressure measurement is performed by measuring the position of R1 ruby flourescence lines as shown in d) for ambient pressure and 17 kbar.

Determining the pressure

Fluorescence, for example, Ruby lines, or other materials





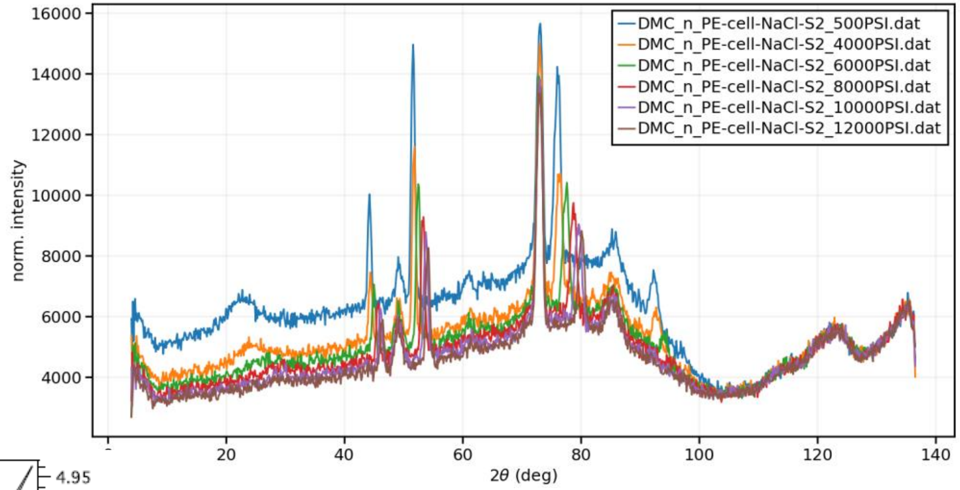


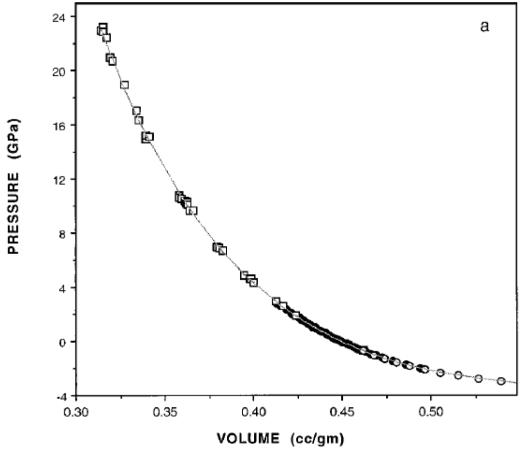
Naumov 2022

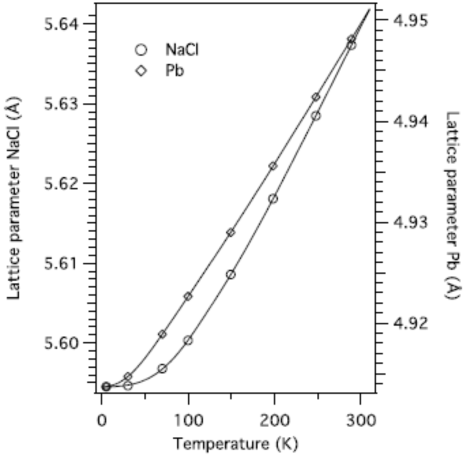
Determining the pressure

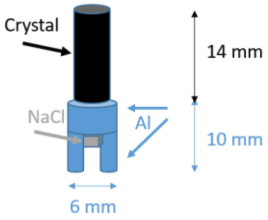
Equation of state:
measure lattice parameters
(and correct for temperature)

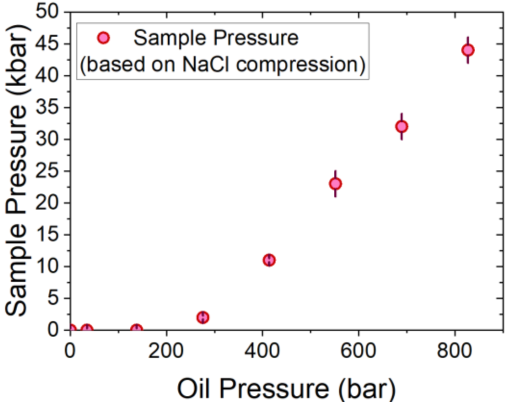
Mixing powder with NaCl or Pb











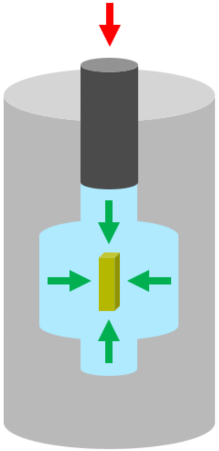
Brown 1999, Strässle 2014

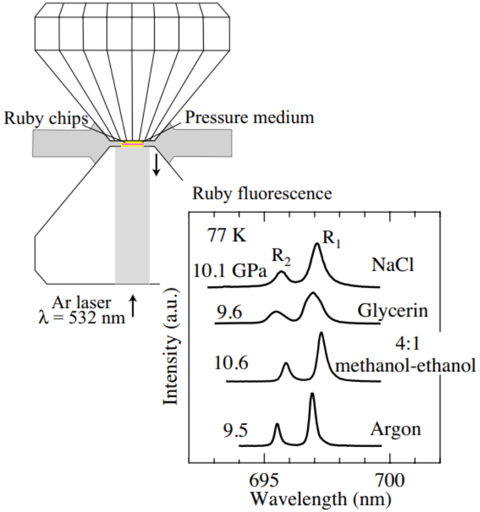
Transmitting the pressure

REVIEW OF SCIENTIFIC INSTRUMENTS **80**, 123901 (2009)

Evaluations of pressure-transmitting media for cryogenic experiments with diamond anvil cell

Naoyuki Tateiwa[a] and Yoshinori Haga





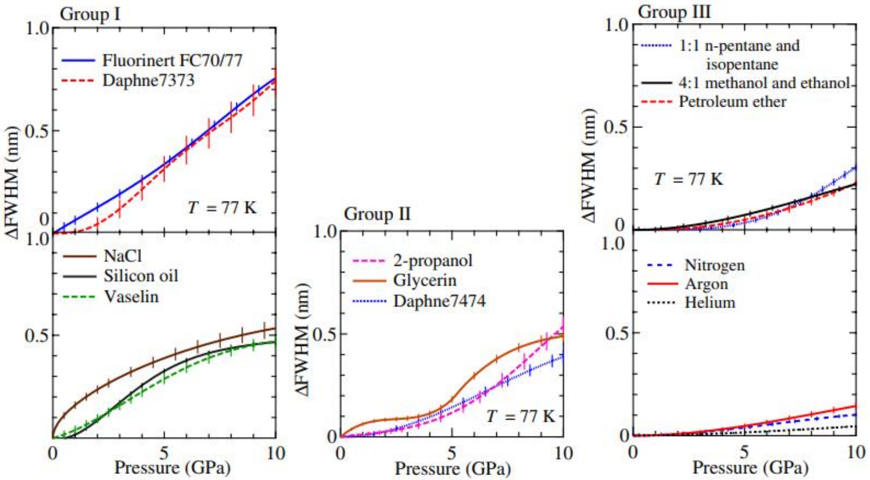


FIG. 7. (Color online) Pressure dependence of ΔFWHM[=FWHM(*P*)−FWHM(0)] of the ruby R_1 line for fourteen pressure media at 77 K. Here, FWHM(*P*) and FWHM(0) are the values of the fitted function for the FWHM under high pressure and ambient pressure, respectively. Error bars indicate averaged deviations of the experimental data of the FWHM from the fitted line at each pressure.

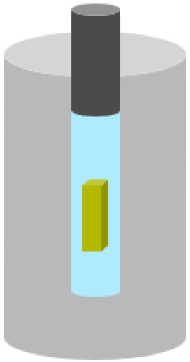
Hydrostaticity difficult to achieve, especially at low-T

Gas medium is the best, but tricky to load

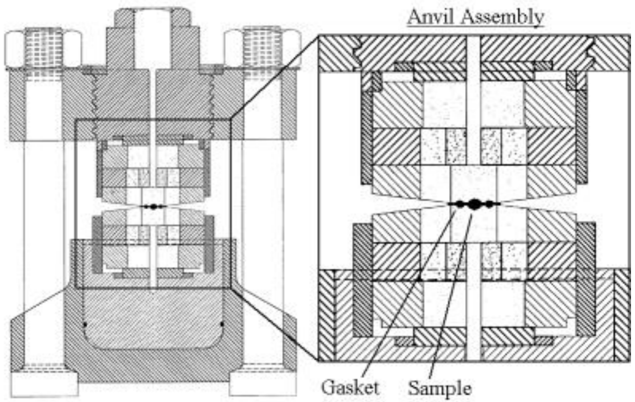
Practical choice – 4:1 methanol ethanol mixture (deuterated)

Thank you for your attention

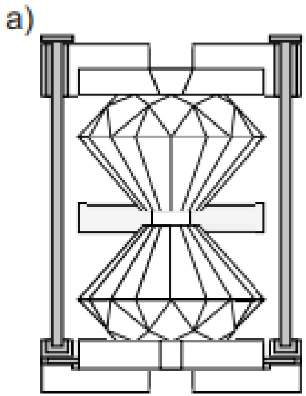
Piston cells



Paris-Edinburgh



DAC



Pressure

Volume

Coming up tomorrow – Uniaxial Pressure, Background Mitigation and MuSR under pressure

Stress-Strain Diagram