Materials Research in Energy Conversion, Storage, and Efficiency

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HiPSEC, University of Nevada Las Vegas

LANSCE, Los Alamos National Laboratory

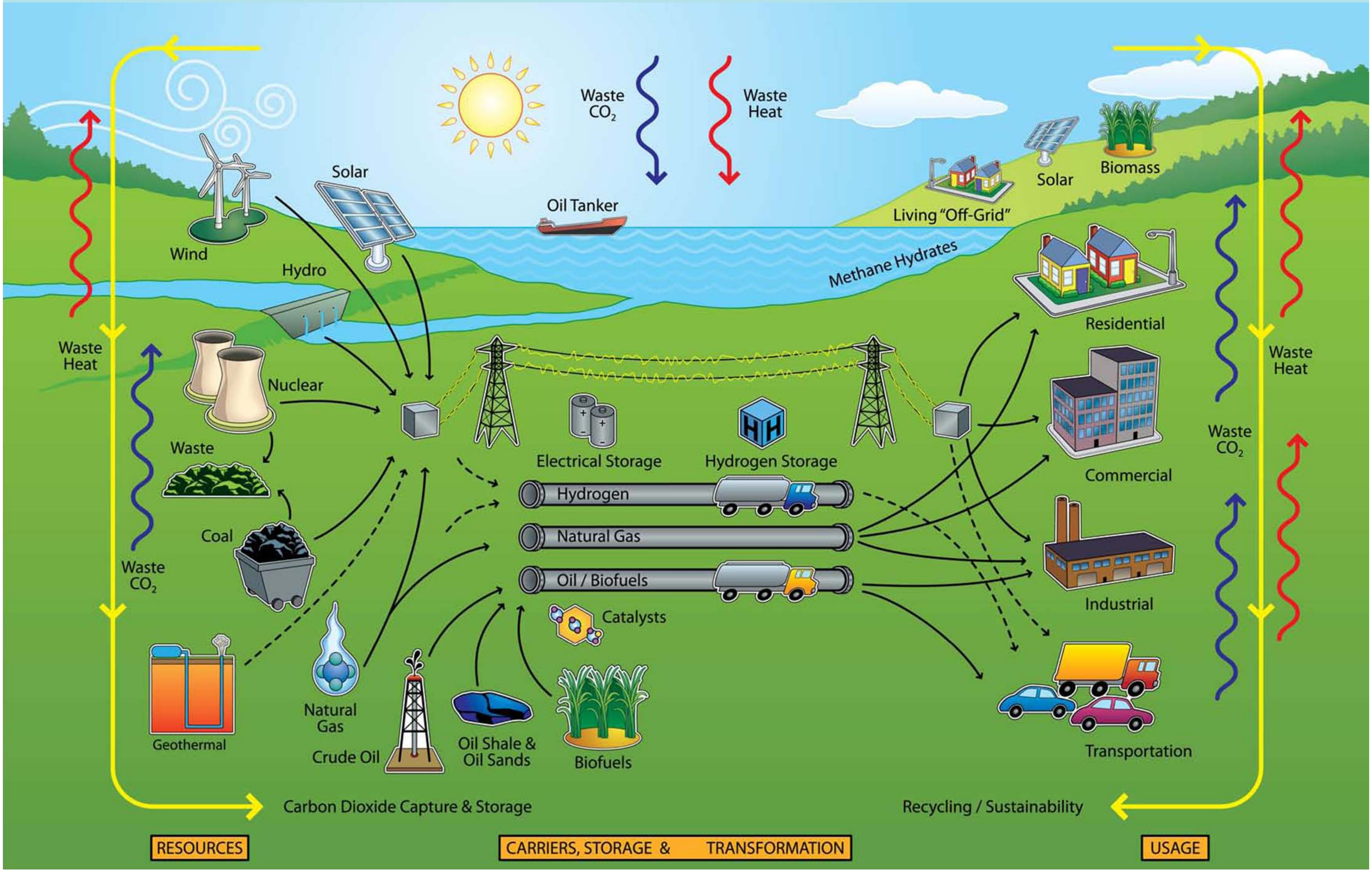
High-Pressure Applications

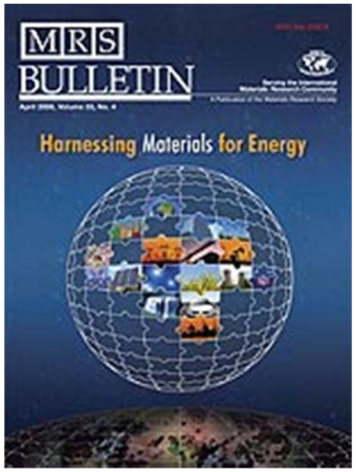
Neutron and Synchrotron X-Ray

Rivalry and Complementary

Harnessing Materials for Energy • MRS BULLETIN • VOLUME 33 • APRIL 2008

Scientific societal efforts reflect the growing global concerns on energy and environment
It also points out the opportunities that materials researchers can take.





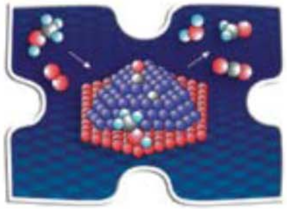
MRS Bulletin
April, 2008

Industrial

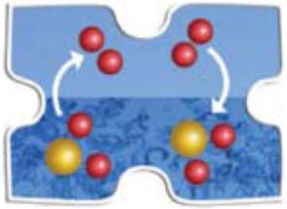
S.S. Lighting

Building

Transportation



Catalysts



Hydrogen

E. Storage

Power Grid

Renewable

Biomass

Solar

Wind

Nuclear

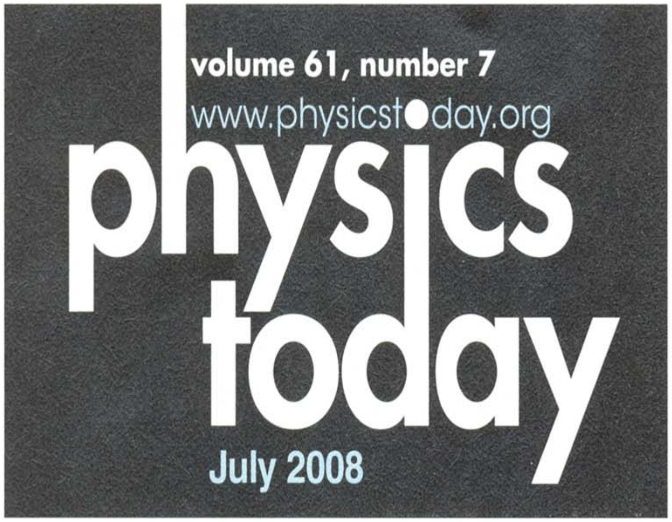
Oil & Gas

Coal

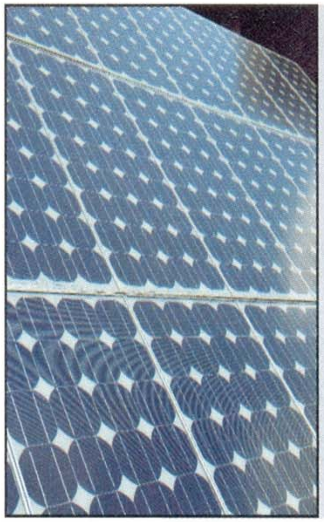
Environment

Economics

Global



volume 61, number 7
www.physicstoday.org
physics today
July 2008

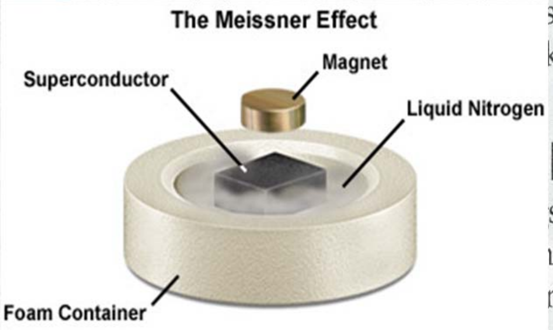


cover: Panels that ge
sunlight—like these i
Maryland—epitomize
of energy consumptio
this issue take close l
fundamental energy-
28), retrofitting of exi
designing of new one
efficiently (page 35),
photovoltaic system (p
the Opinion piece on
the need for an educ
scientists can help. (P
and Bill Koplitz.)

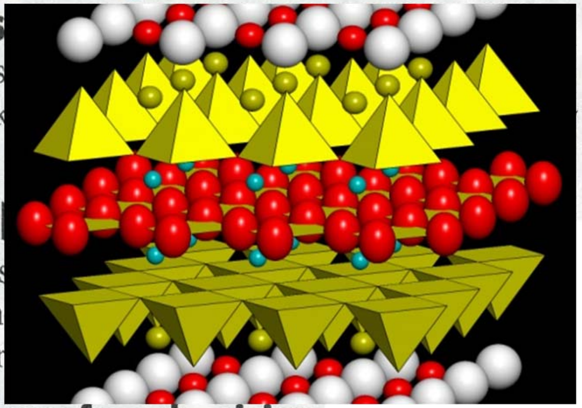
feature articles

Special focus: Energy today and tomorrow

28 Grand challenges in bas



The Meissner Effect



42 Home photovoltaic systems for physicists

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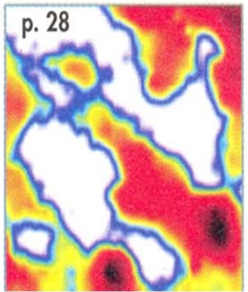
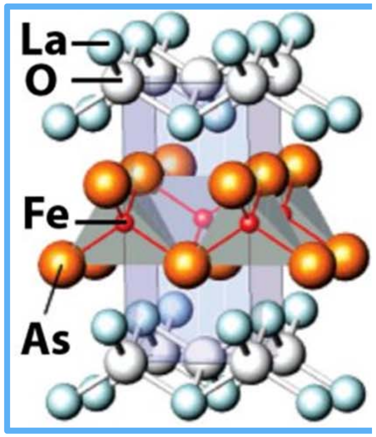
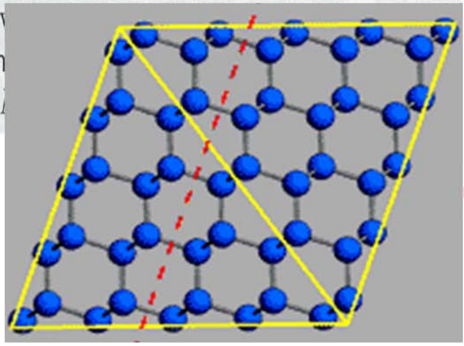
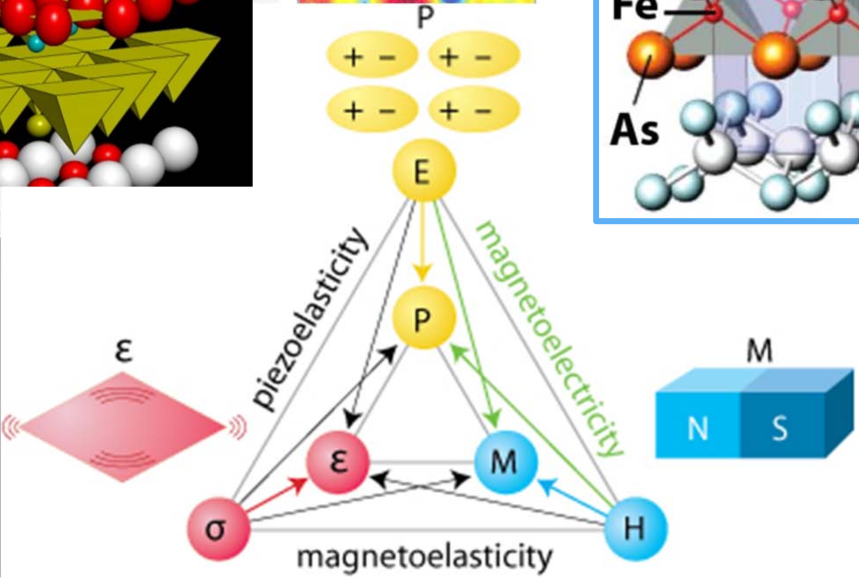




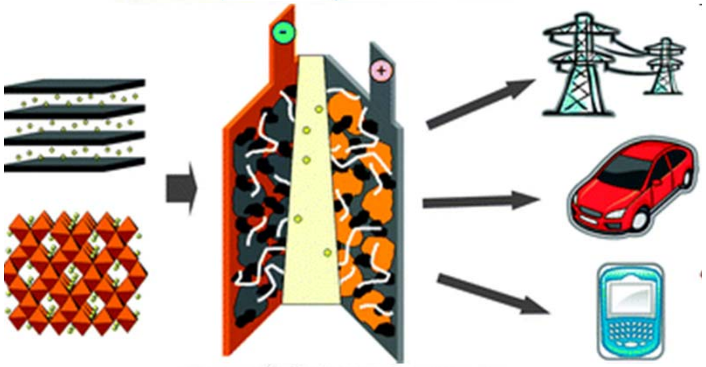




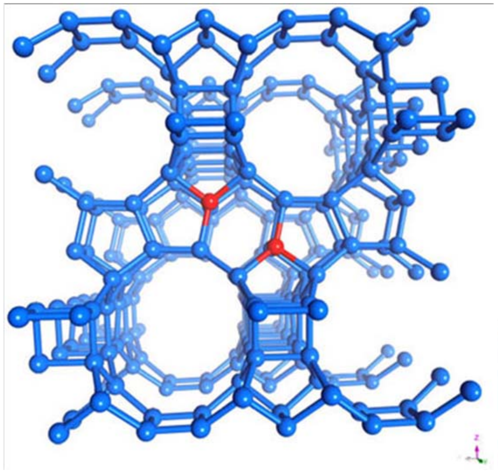
4th International ology Symposium

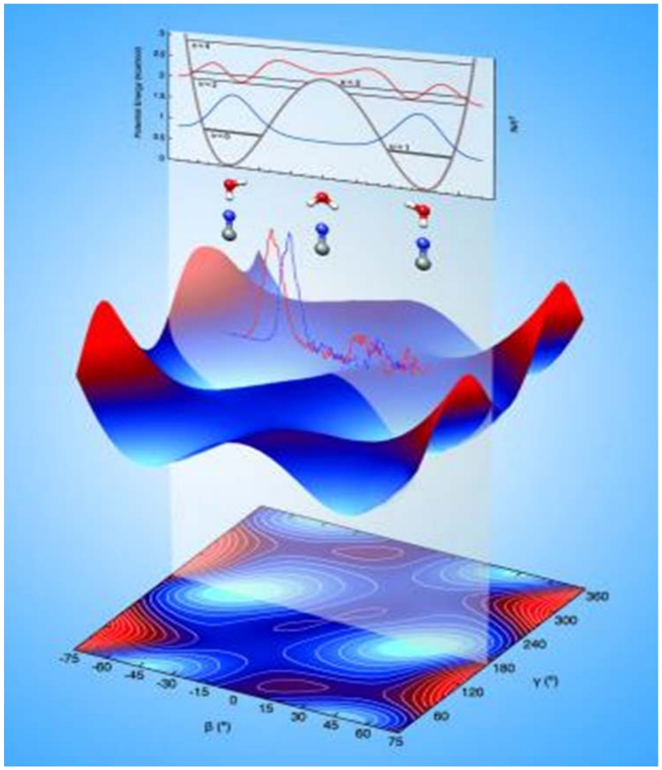
239th American National Meeting

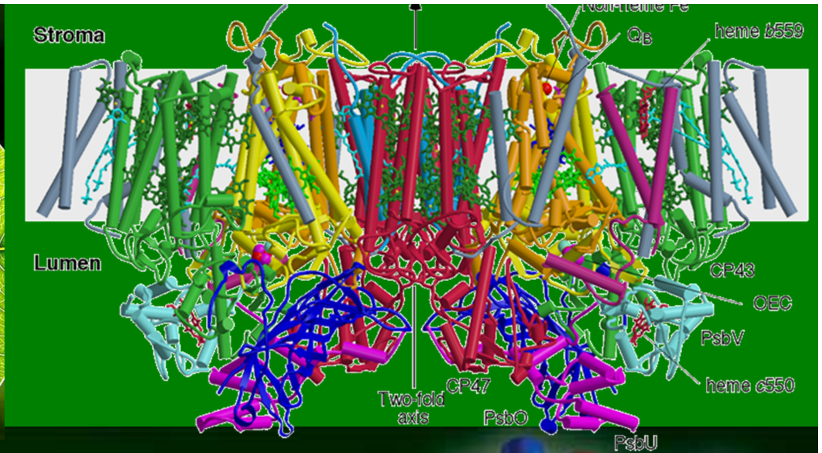
San Francis March 2010

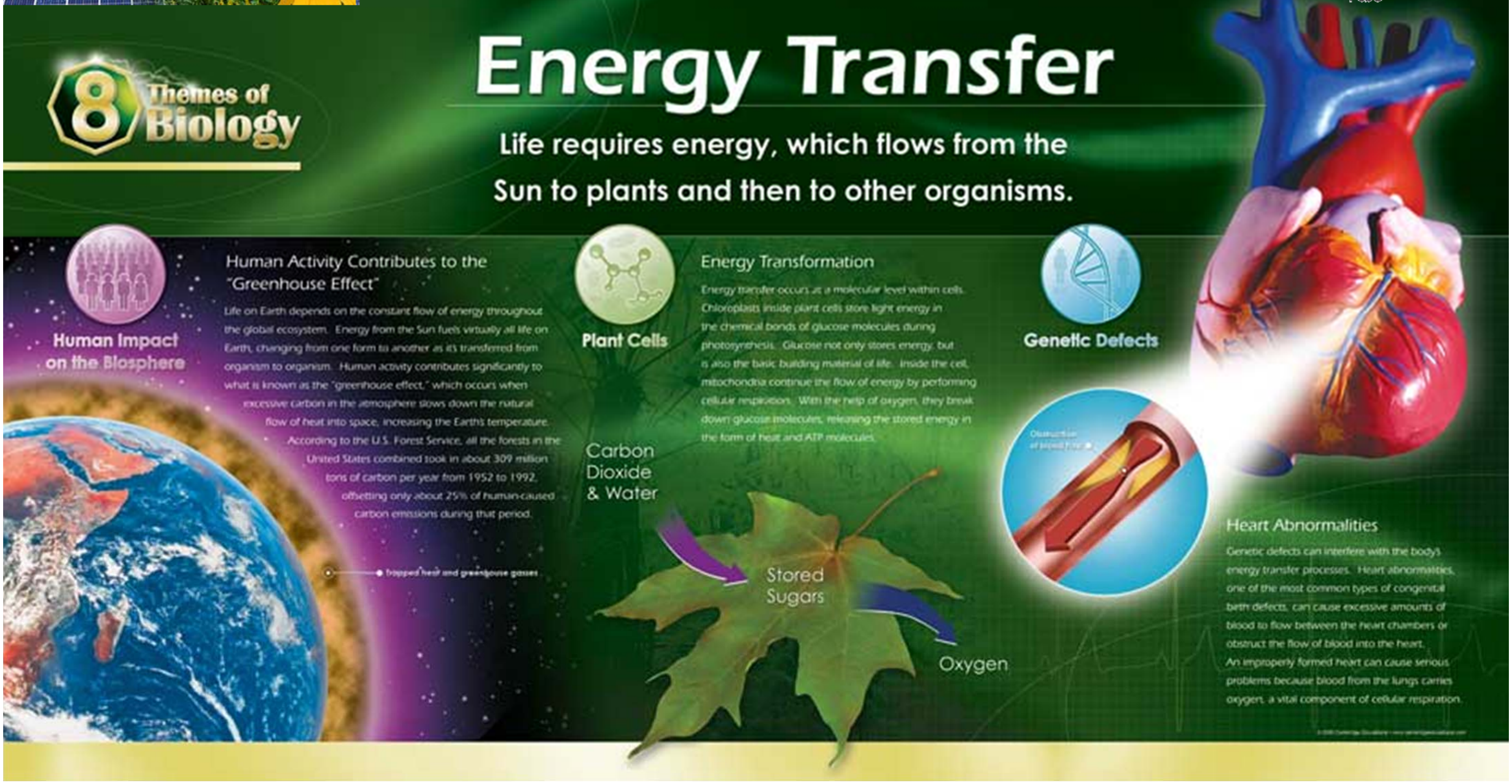


- Low-Energy Nuclear Reaction Research
  - Other new energy technologies
  - Energy Sustainability Concepts









Energy Transfer

Life requires energy, which flows from the Sun to plants and then to other organisms.

Human Impact on the Biosphere

Human Activity Contributes to the "Greenhouse Effect"

Life on Earth depends on the constant flow of energy throughout the global ecosystem. Energy from the Sun fuels virtually all life on Earth, changing from one form to another as it's transferred from organism to organism. Human activity contributes significantly to what is known as the "greenhouse effect," which occurs when excessive carbon in the atmosphere slows down the natural flow of heat into space, increasing the Earth's temperature. According to the U.S. Forest Service, all the forests in the United States combined took in about 309 million tons of carbon per year from 1952 to 1992, offsetting only about 25% of human-caused carbon emissions during that period.

Plant Cells

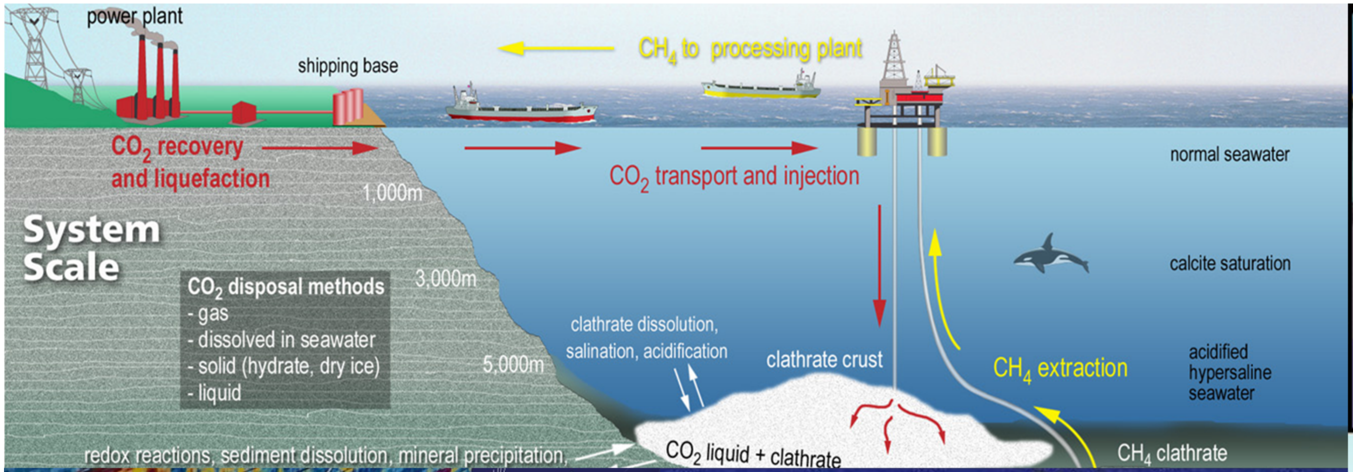
Energy Transformation

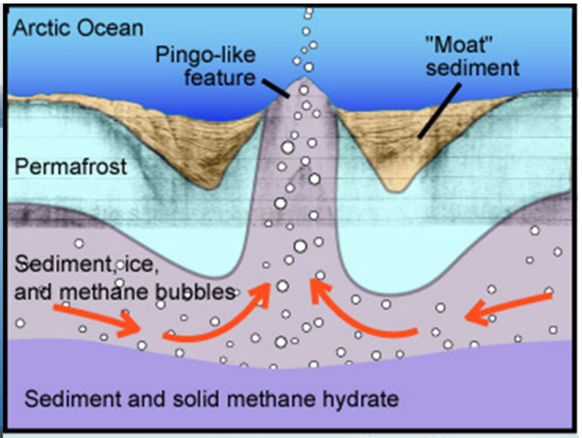
Energy transfer occurs at a molecular level within cells. Chloroplasts inside plant cells store light energy in the chemical bonds of glucose molecules during photosynthesis. Glucose not only stores energy, but is also the basic building material of life. Inside the cell, mitochondria continue the flow of energy by performing cellular respiration. With the help of oxygen, they break down glucose molecules, releasing the stored energy in the form of heat and ATP molecules.

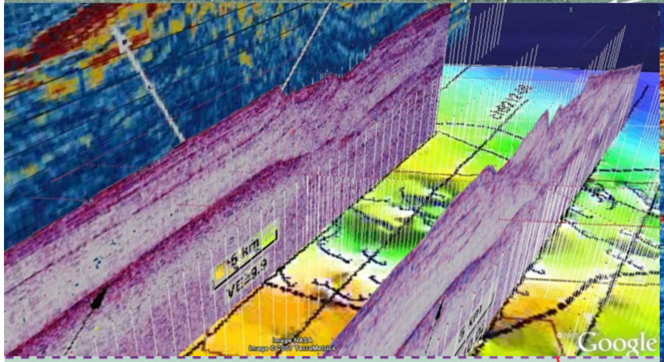
Genetic Defects

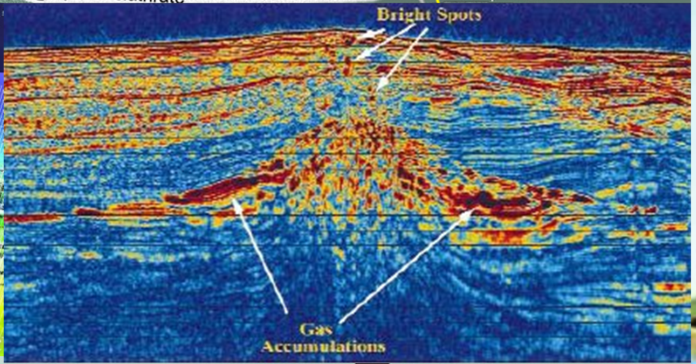
Heart Abnormalities

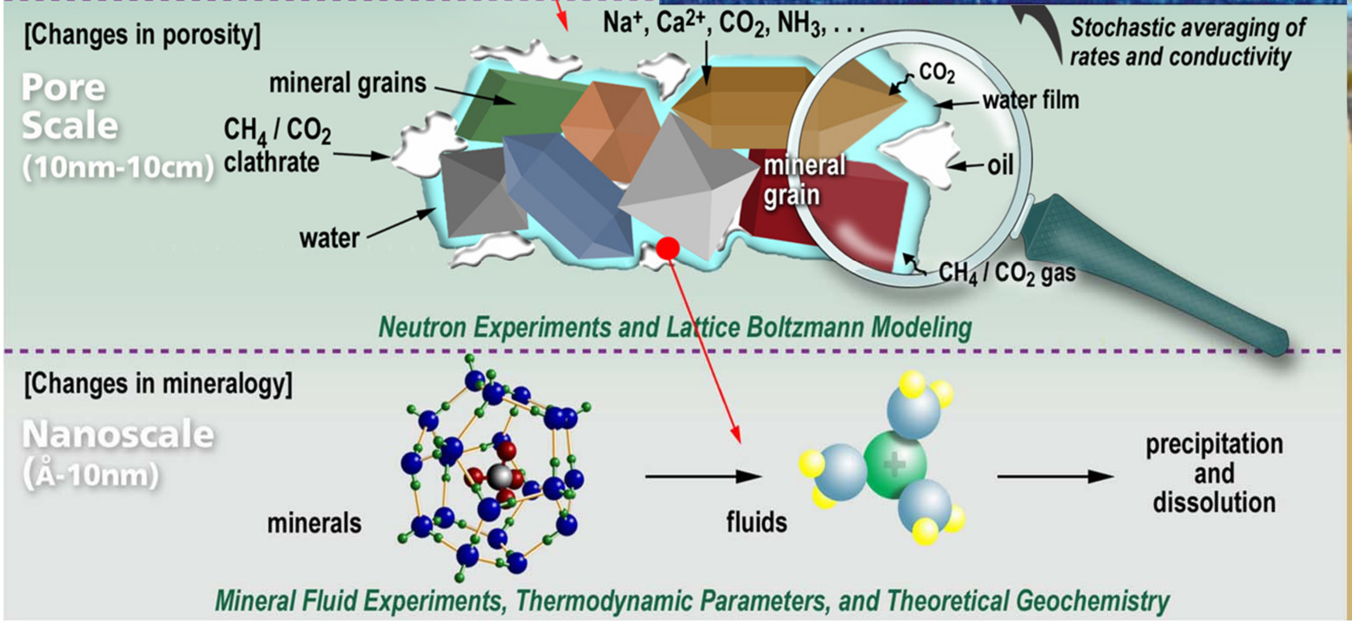
Genetic defects can interfere with the body's energy transfer processes. Heart abnormalities, one of the most common types of congenital birth defects, can cause excessive amounts of blood to flow between the heart chambers or obstruct the flow of blood into the heart. An improperly formed heart can cause serious problems because blood from the lungs carries oxygen, a vital component of cellular respiration.

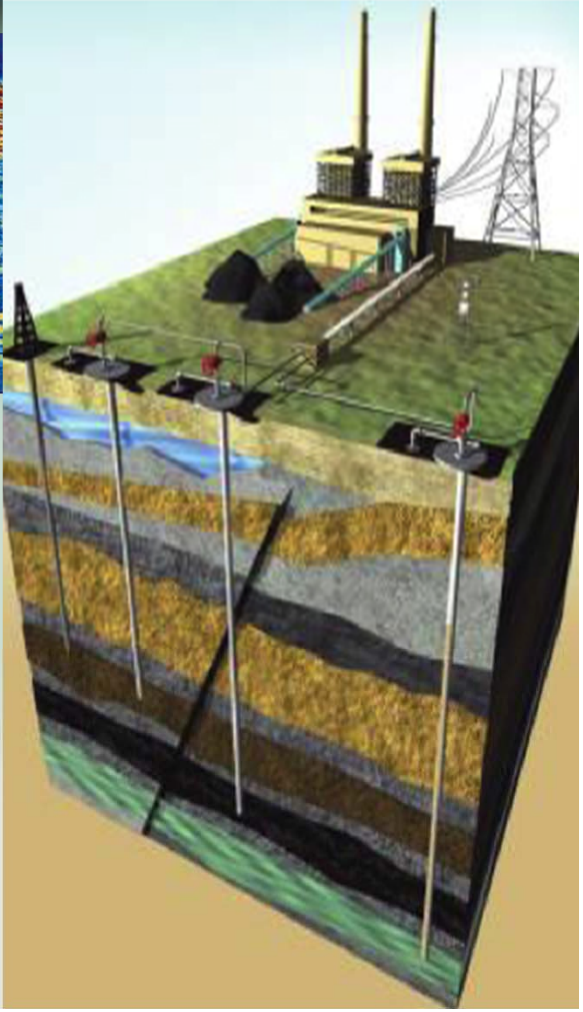

power plant
shipping base
CH_4 to processing plant
CO_2 recovery and liquefaction
CO_2 transport and injection
normal seawater
1,000m
System Scale
3,000m
calcite saturation
CO_2 disposal methods
- gas
- dissolved in seawater
- solid (hydrate, dry ice)
- liquid
5,000m
clathrate dissolution, salination, acidification
clathrate crust
CH_4 extraction
acidified hypersaline seawater
redox reactions, sediment dissolution, mineral precipitation,
CO_2 liquid + clathrate
CH_4 clathrate

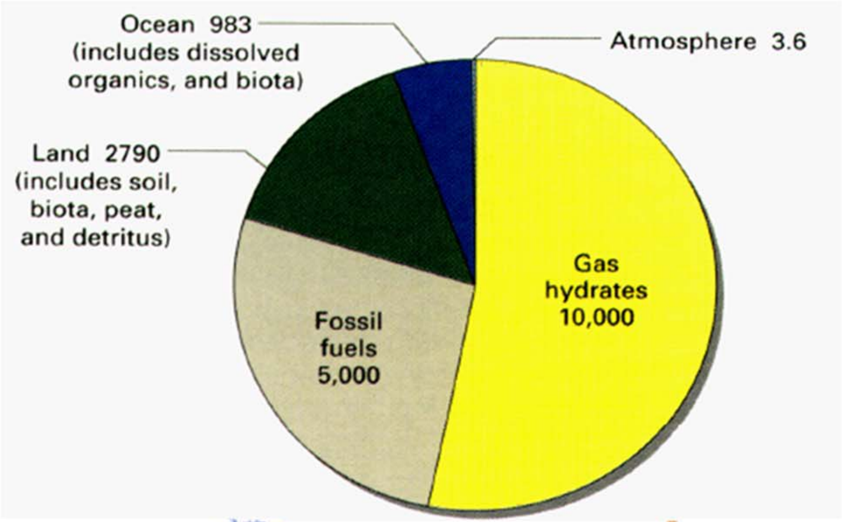

Arctic Ocean
Pingo-like feature
"Moat" sediment
Permafrost
Sediment, ice, and methane bubbles
Sediment and solid methane hydrate


5 km
VE=9.9
Google


Bright Spots
Gas Accumulations


[Changes in porosity]
Na^+, Ca^{2+}, CO_2, NH_3, . . .
Stochastic averaging of rates and conductivity
Pore Scale (10nm-10cm)
mineral grains
CO_2
water film
CH_4 / CO_2 clathrate
mineral grain
oil
water
CH_4 / CO_2 gas
Neutron Experiments and Lattice Boltzmann Modeling
[Changes in mineralogy]
Nanoscale (Å-10nm)
minerals
fluids
precipitation and dissolution
Mineral Fluid Experiments, Thermodynamic Parameters, and Theoretical Geochemistry





Methane Hydrate Drill-Core

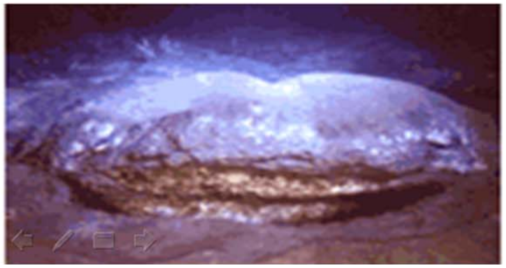
En modifiant la densité de l'eau, les bulles de gaz qui s'échappent des sédiments feraient chavirer les bateaux.

A 3 km au large d'Hawaii, un bateau injectera à 800 m de profondeur du dioxyde de carbone liquide, à une pression de 80 bars et une température de 5 °C.

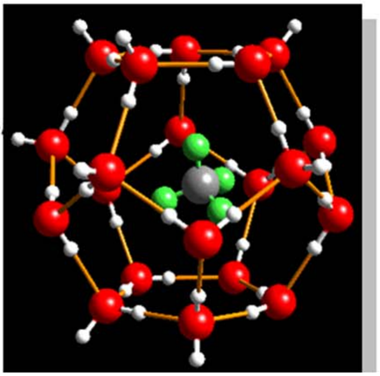
CH_4-H_2O Worldwide Deposits

Mystery of Bermuda Triangle

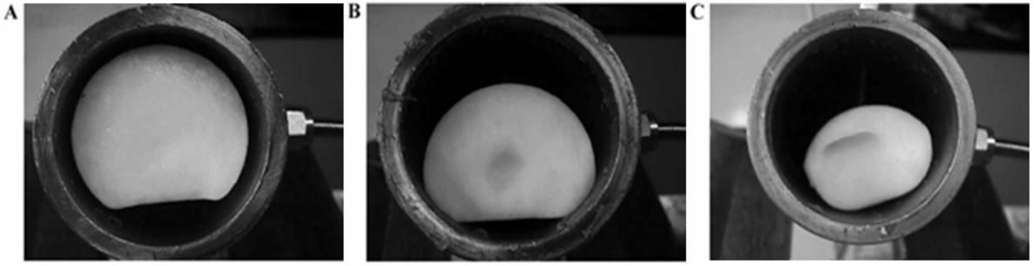
"Burning Ice"

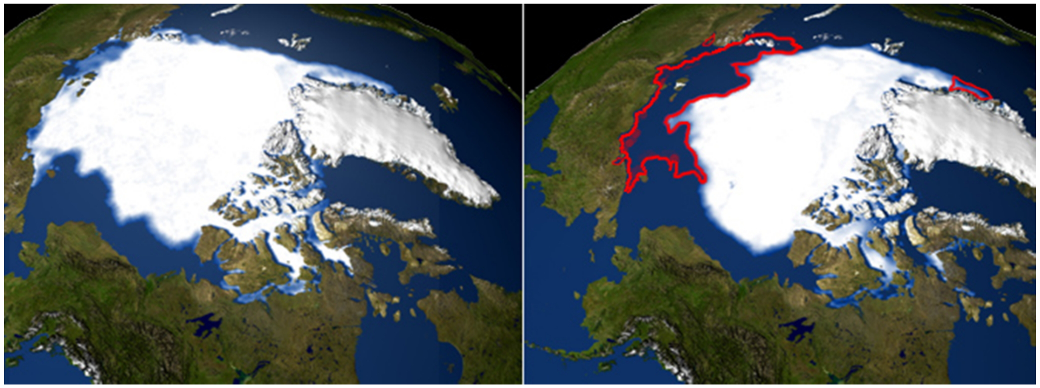


Methane Hydrate Wo

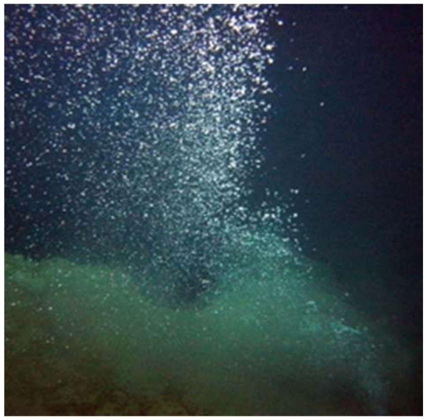


Pipeline Safety!

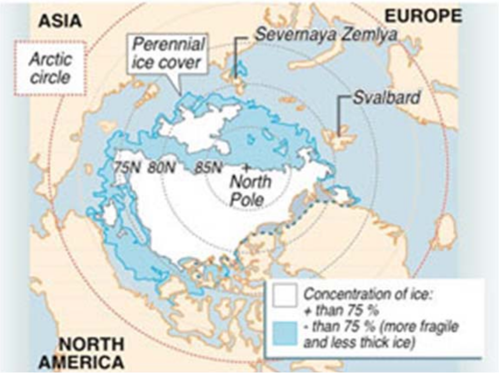


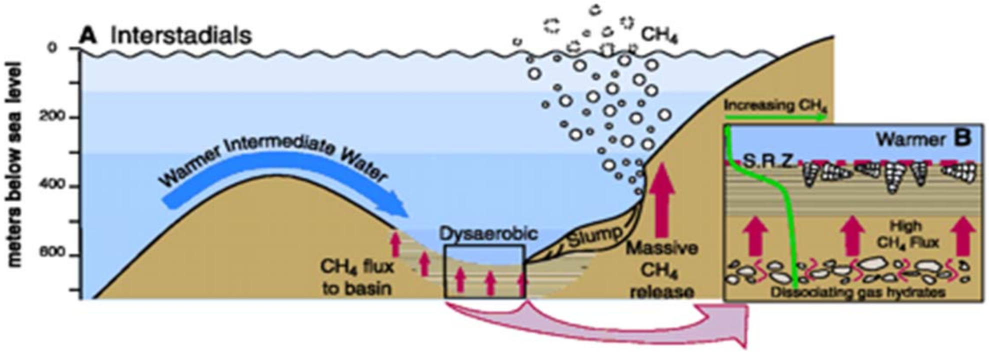


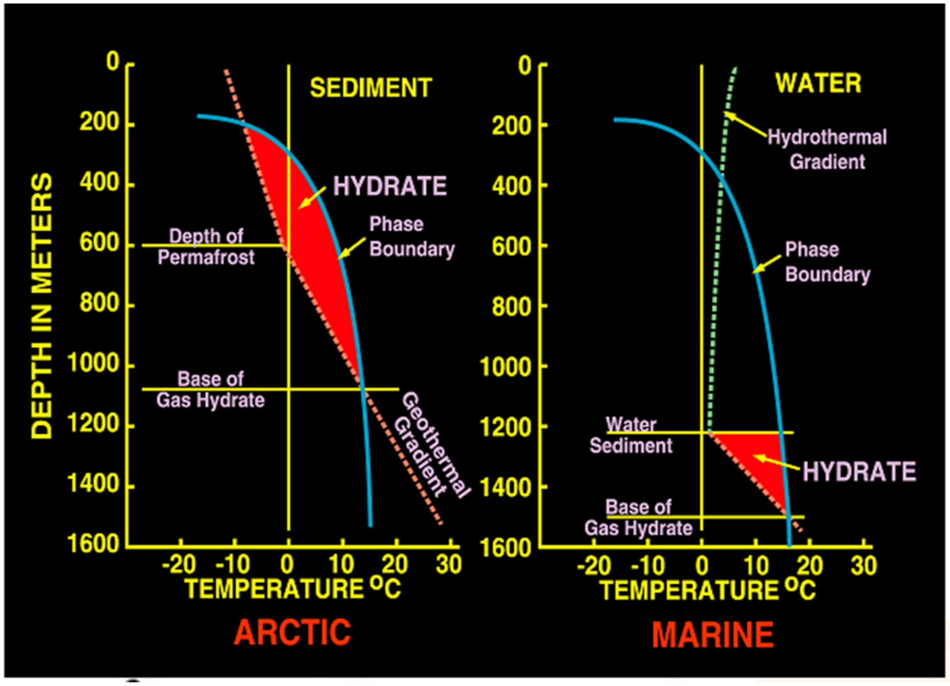
Bubbling Out CH_4/CO_2 due to Hydrates Breakdown

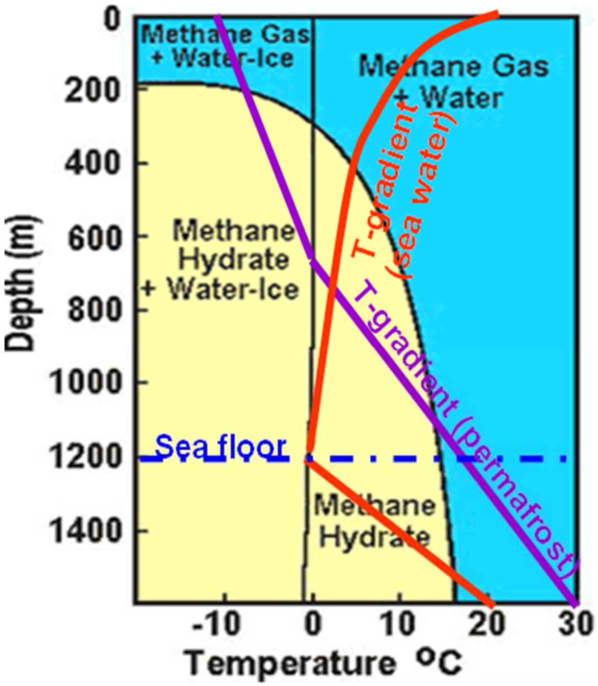


Global Warming Impact on Hydrate Deposits









1 m^3 $CH_4 \cdot H_2O$

Contains

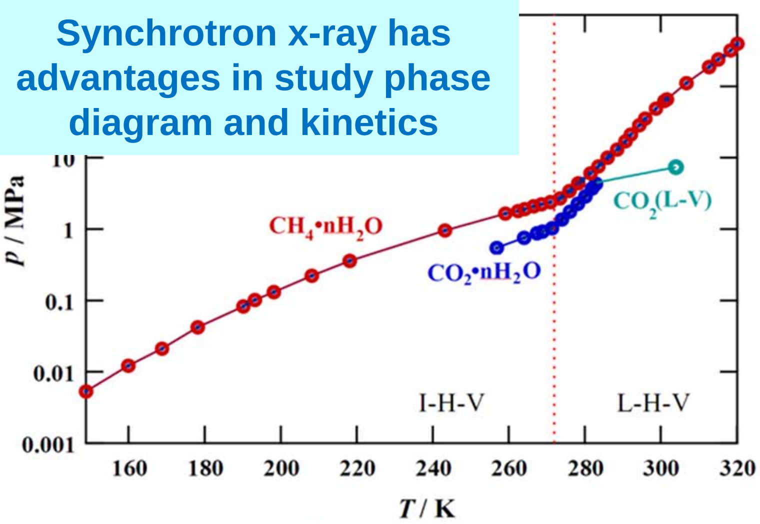
164 m^3 CH_4

SI clathrate

2 x 5^{12}

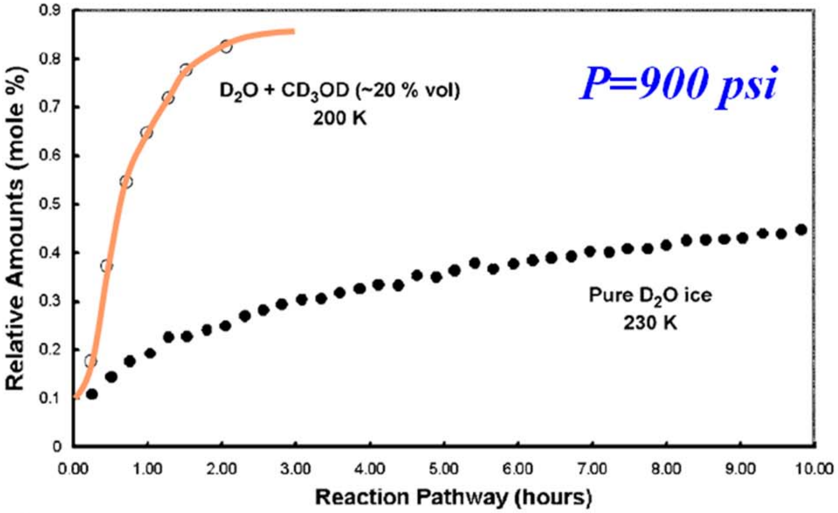
6 x $5^{12}6^2$

Synchrotron x-ray has advantages in study phase diagram and kinetics

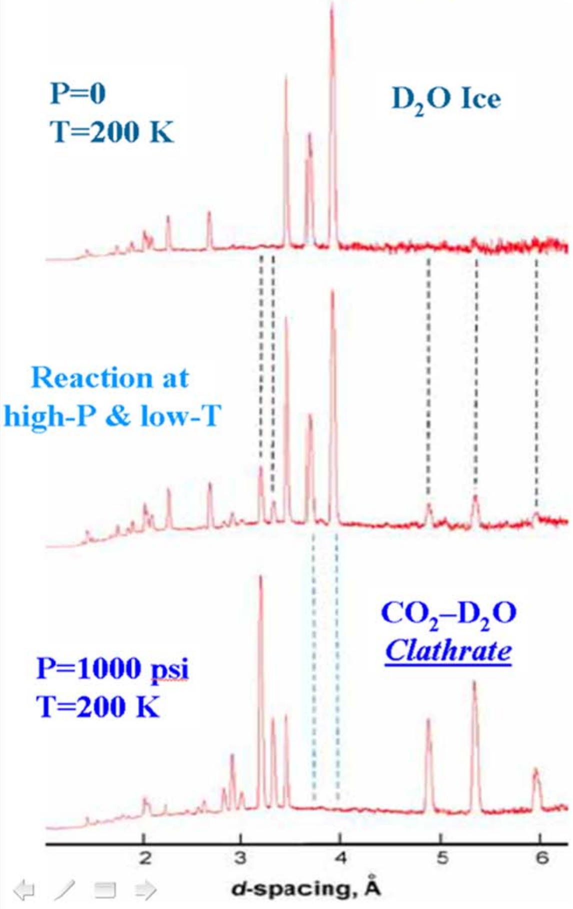


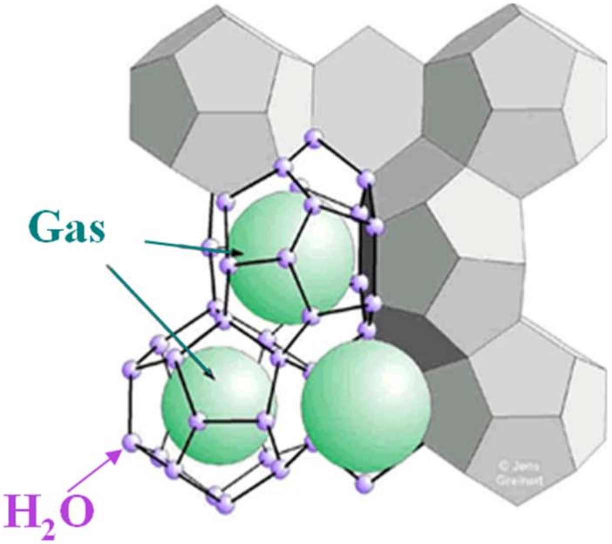
Thermodynamics

Kinetics



P=900 psi

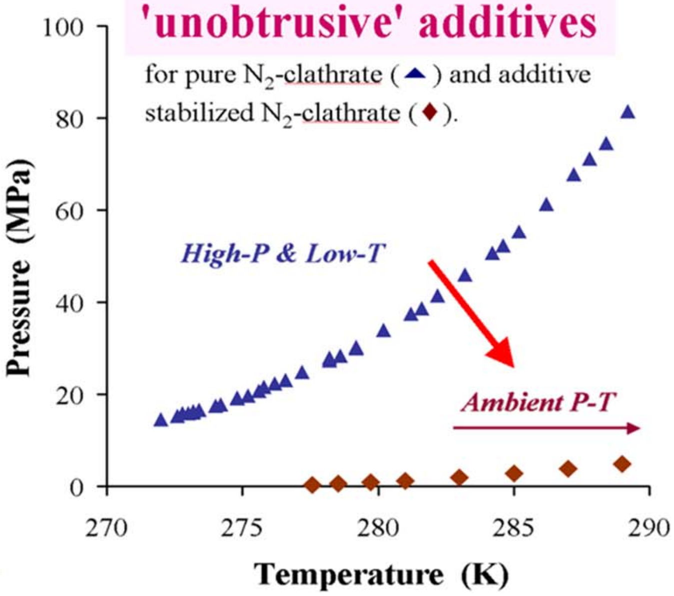




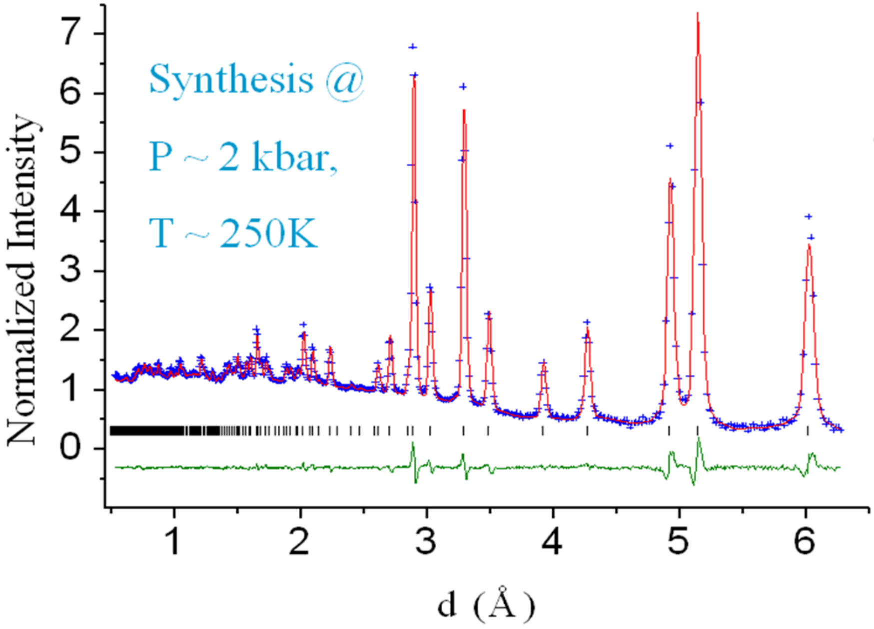
Formation kinetics of CO_2-H_2O clathrate hydrate observed *in-situ* & *real-time* by high-*P* low-*T* neutron diffraction

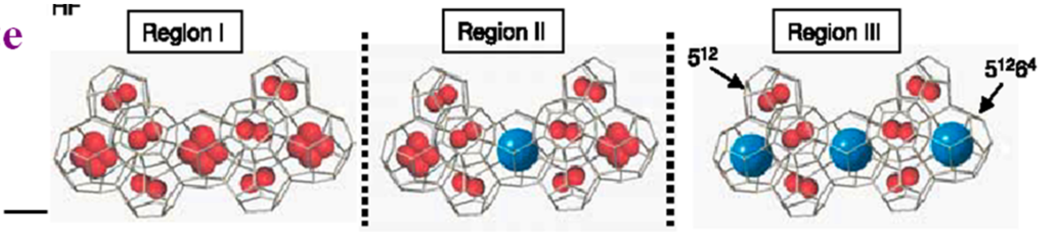
The addition of methanol greatly increase the rate of formation of CO_2-hydrate!

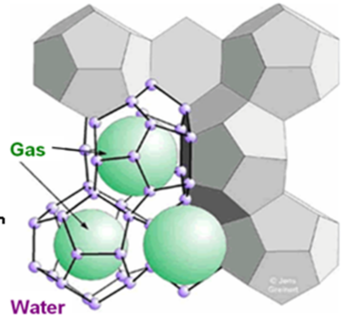
'unobtrusive' additives



Neon : cubic structure II clathrate hydrate

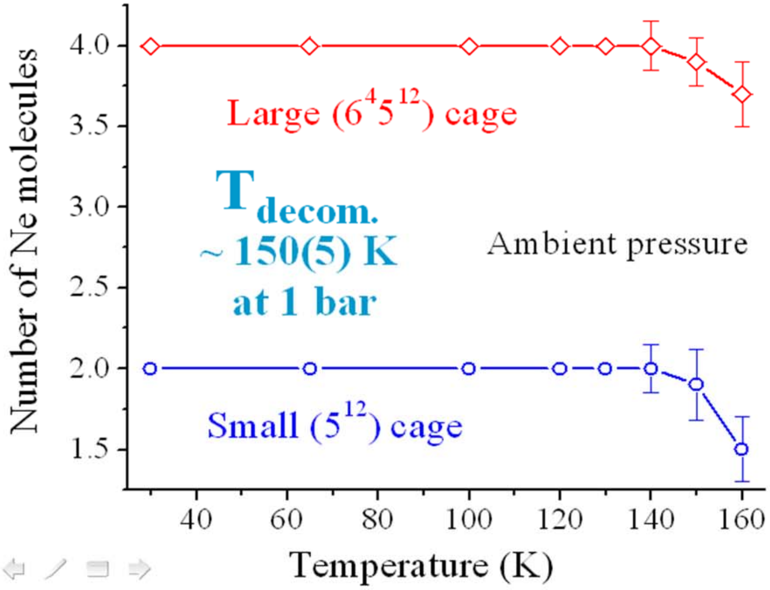


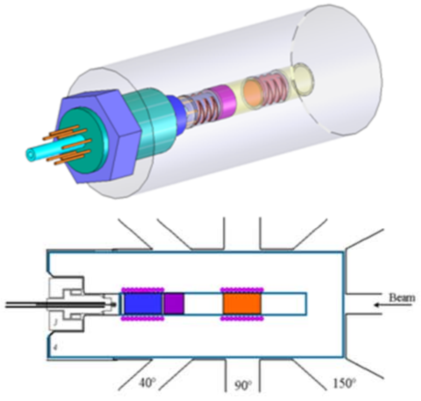




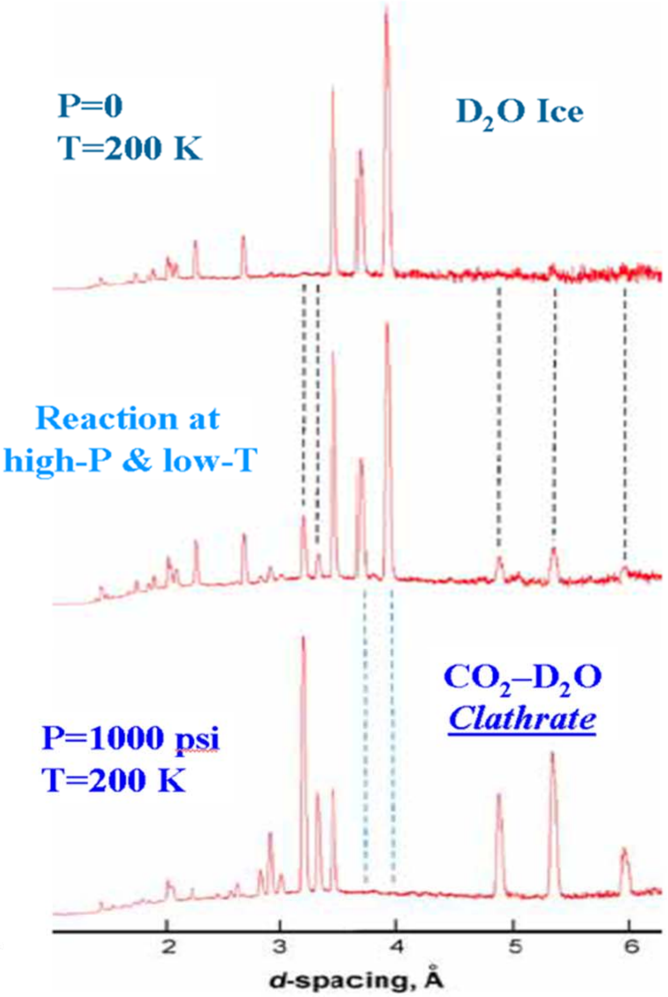
Formation kinetics of CO_2-H_2O clathrate hydrate observed *In-situ* & *real-time* by high-P low-T neutron diffraction

$64Ne*136D_2O \rightarrow 4 \times 8\ \{5^{12}6^4\} + 2 \times 16\ \{5^{12}\}$



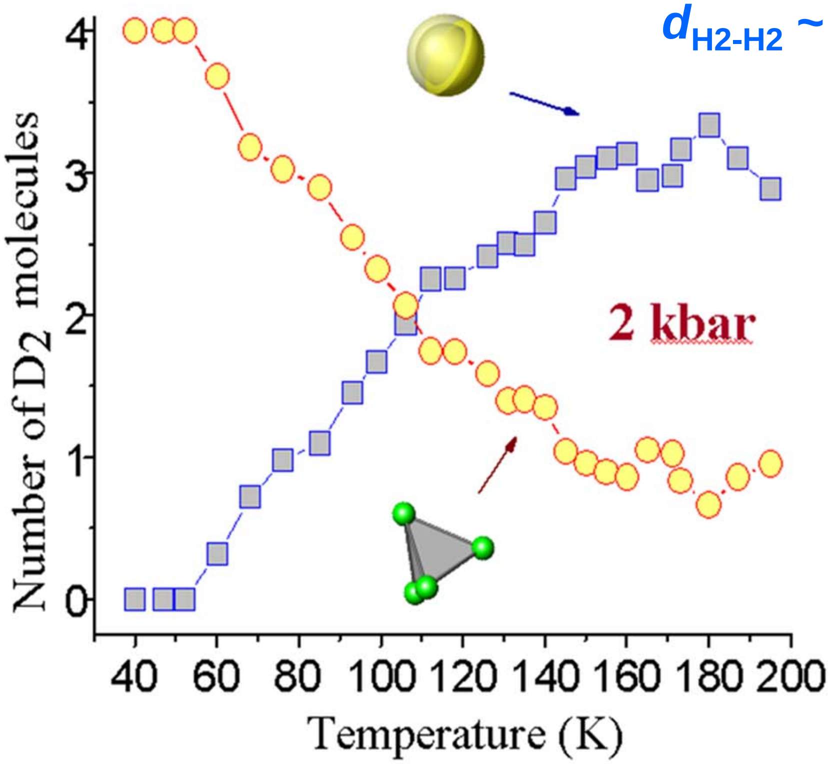


Diffraction + Calorimetry

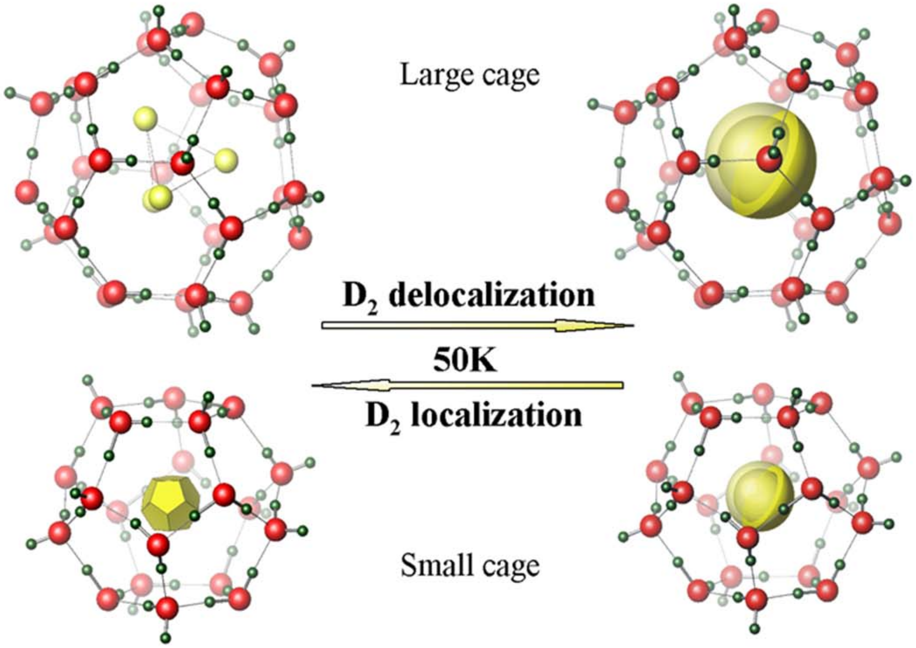


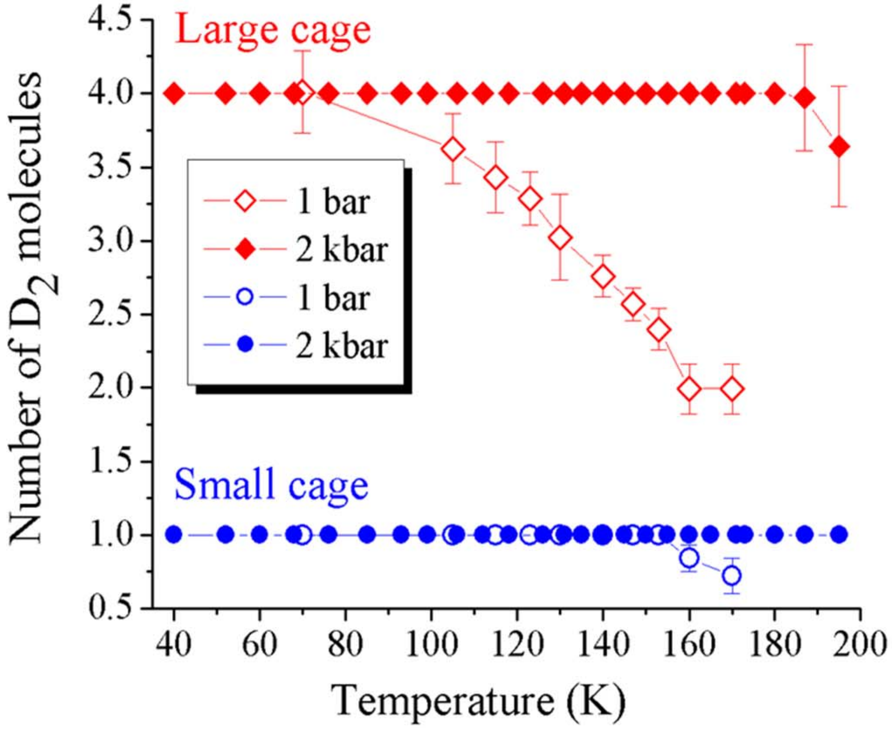
Tech Integration

Hydrogen distribution refined as a linear combination of ***localized*** and ***delocalized*** models

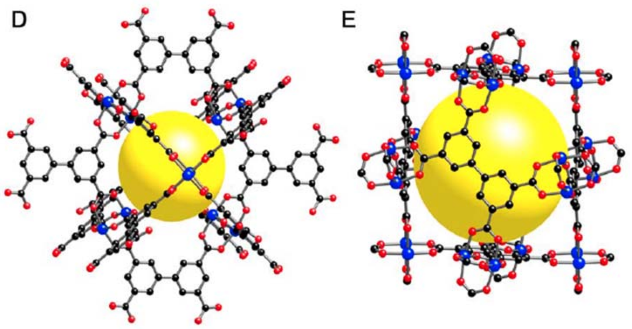


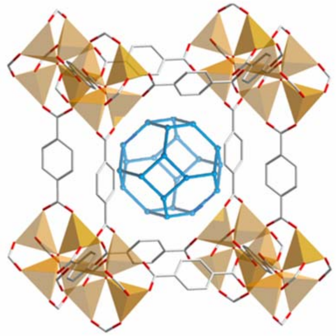
$d_{H2\text{-}H2}$ ~ 2.9 Å

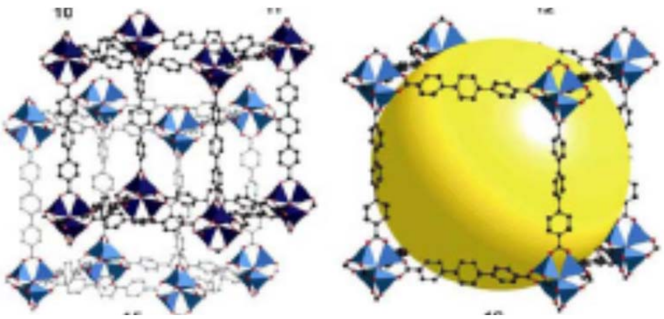




Neutron has advantages in refining the crystal structure and molecular encapsulations as function of pressure and temperature for clathrate hydrates

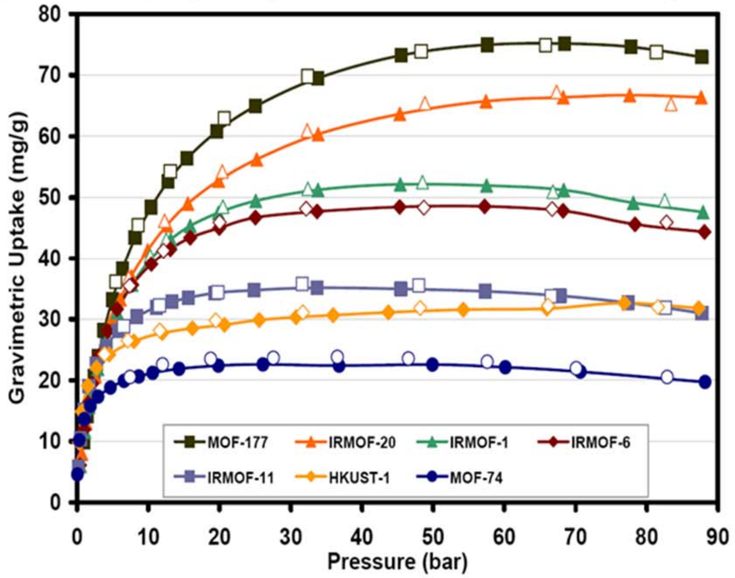


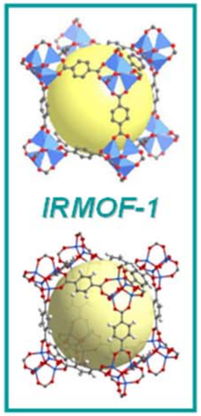




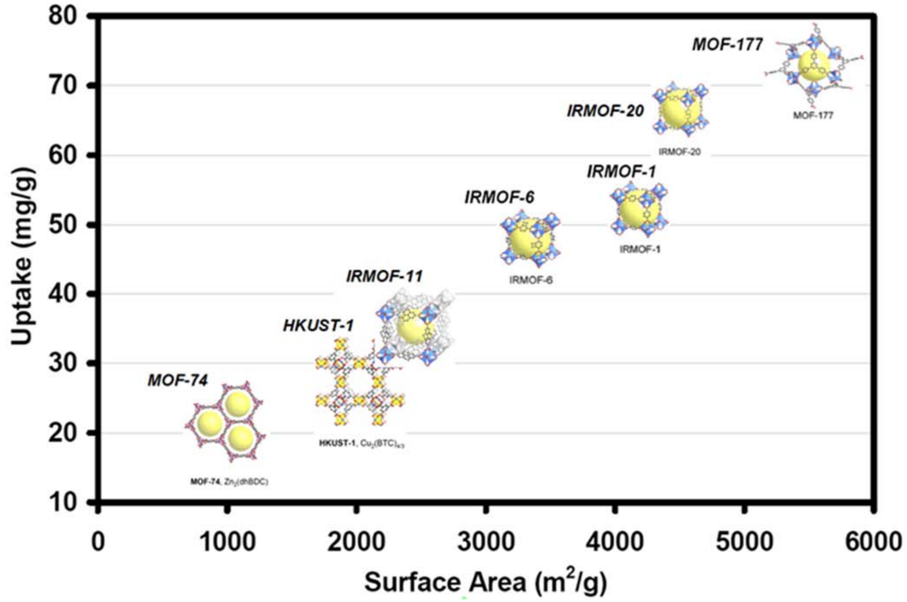
Gas Adsorption

Hydrogen uptake at 77 K





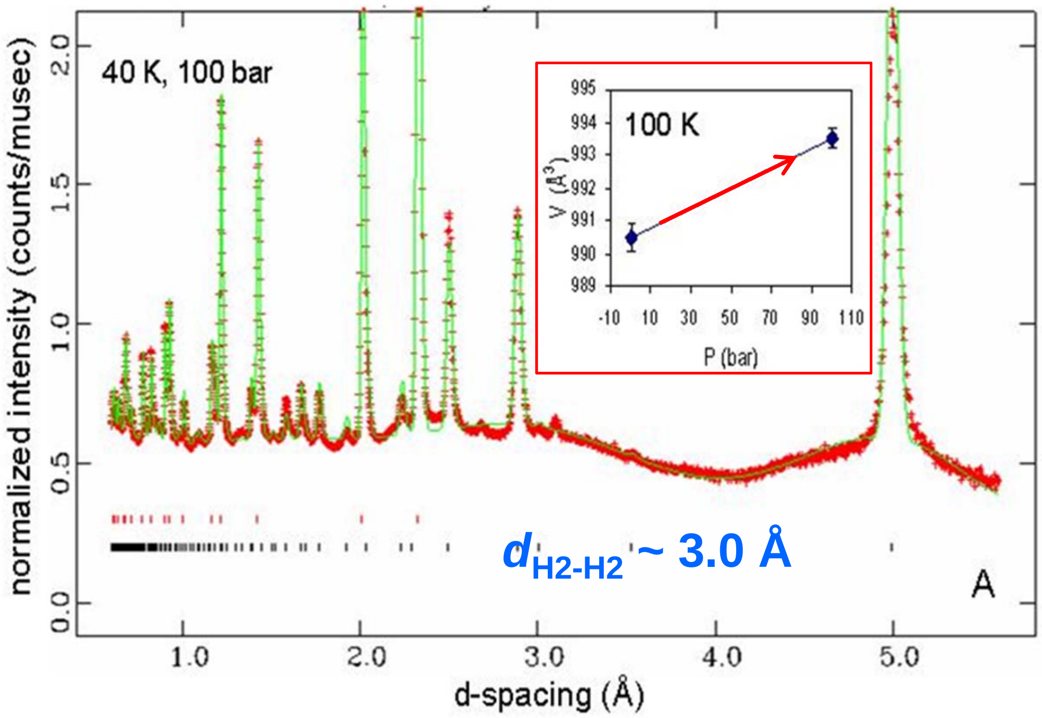
Correlation of uptake with surface area



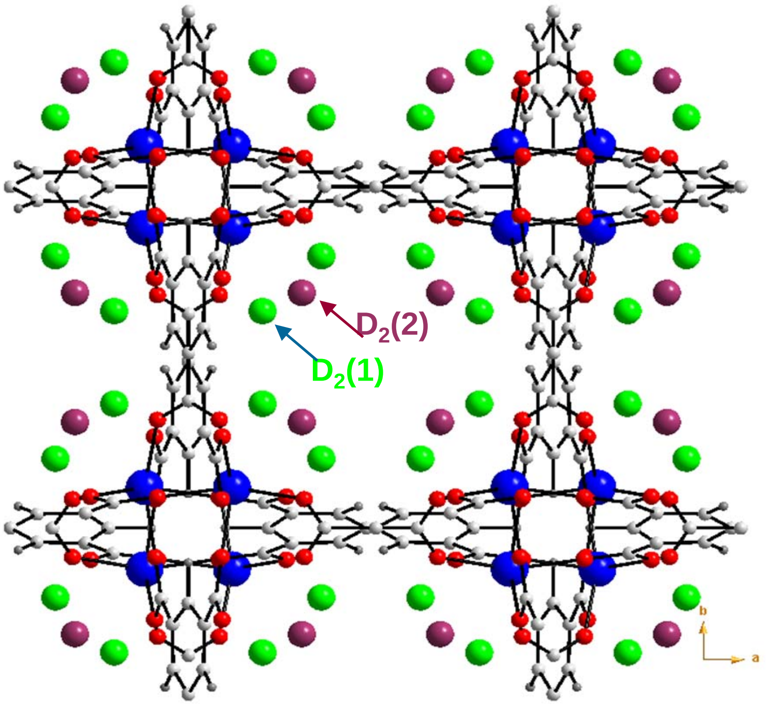
The metal-organic framework (MOF)

Y(BTC)(H2O)·4.3H2O (BTC = 1,3,5-benzenetricarboxylate) for the present case.

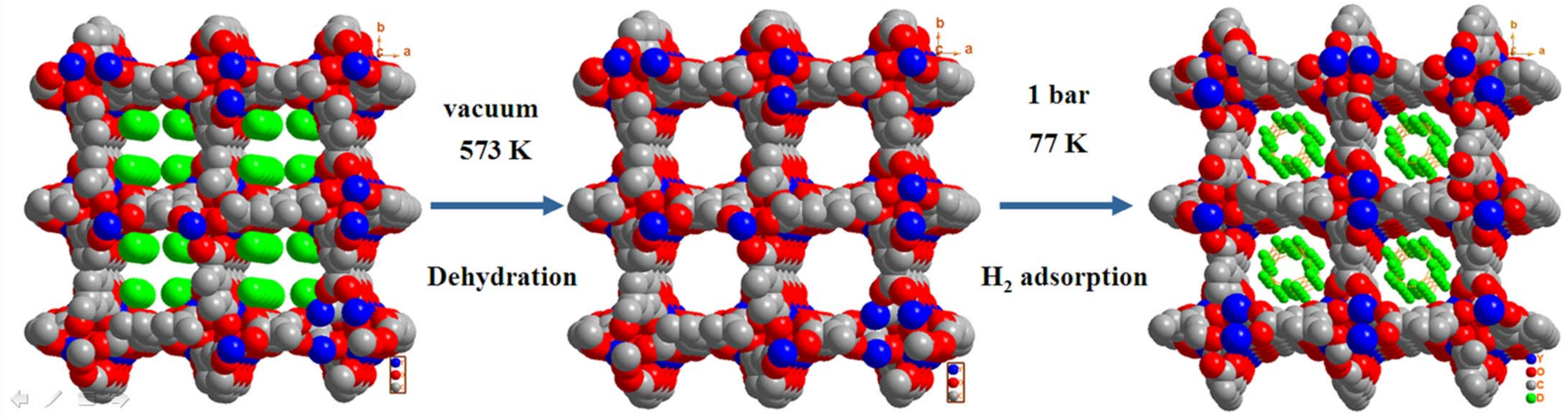
MOFs show striking pressurizing effect by the cages. Owing to the enormous variety and flexibility of the frameworks, MOFs may offer superior properties for hydrogen storage.



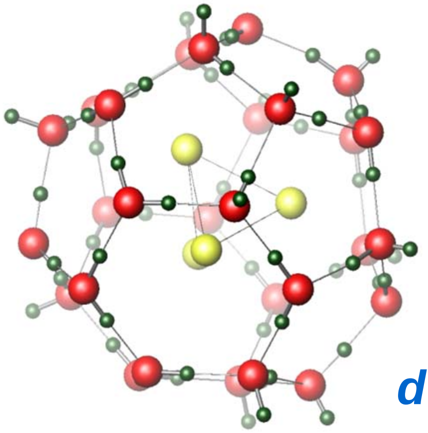
$d_{H2\text{-}H2}$ ~ 3.0 Å



high-*P* / low-*T* neutron diffraction to reveal H_2 adsorption mechanism



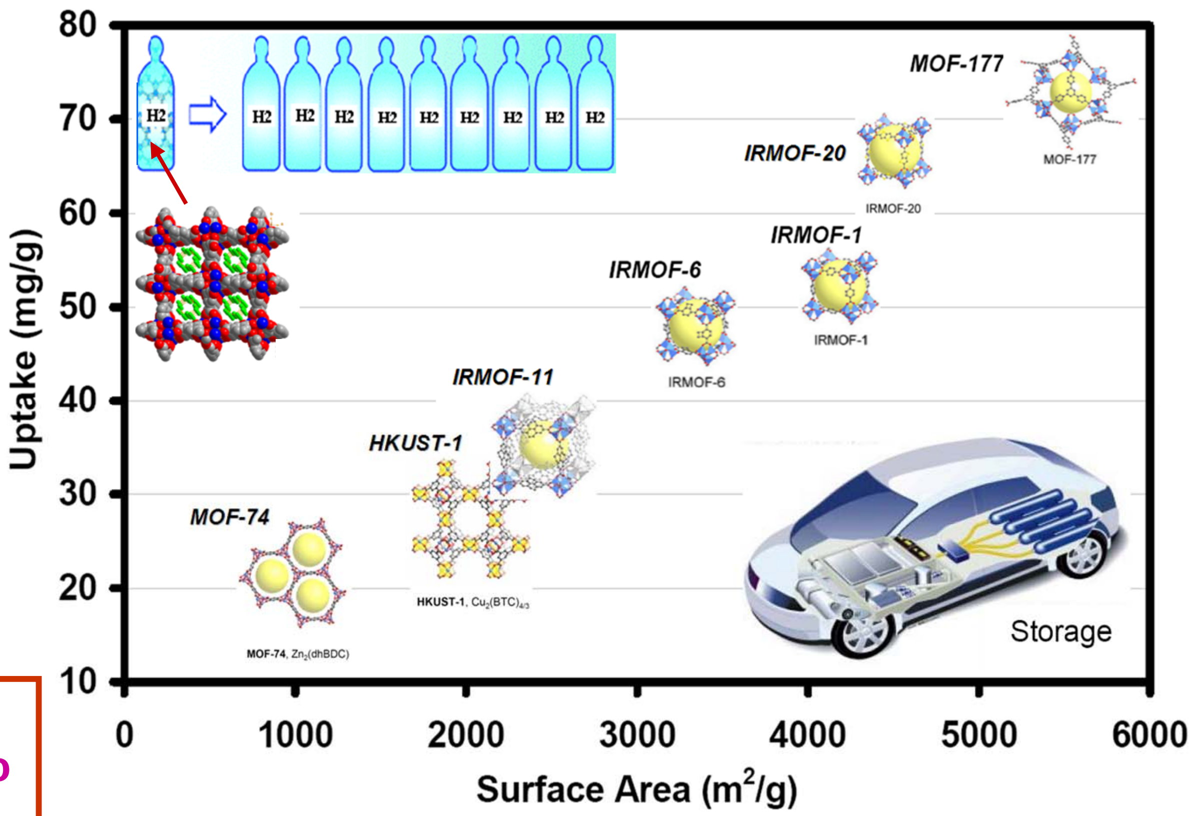
host-guest interactions (quantum clustering)



Hydrogen Clathrate Hydrate

Cage Structure

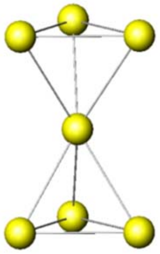
$d_{H2\text{-}H2} \sim 2.9$ Å



20~22% reduction of the bond length in *hydrogen cluster* need to apply as much as 10's kbar in pressure !!!

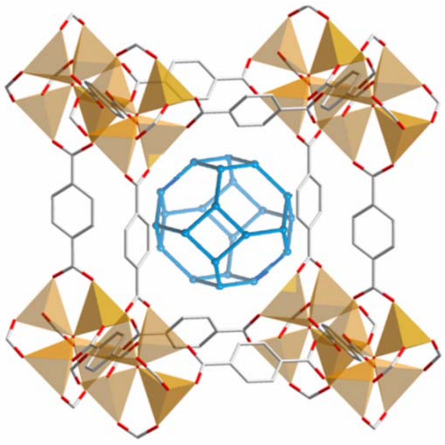
$d_{H2\text{-}H2} \sim 3.76$ Å

$d_{H2\text{-}H2} \sim 3.0$ Å



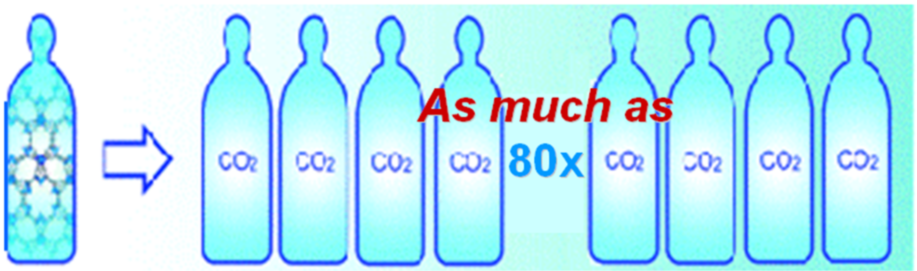
Solid Hydrogen

Metal-Organic Framework



The host nano-encapsulation shows strong ***pressurizing*** effects applied on the guest

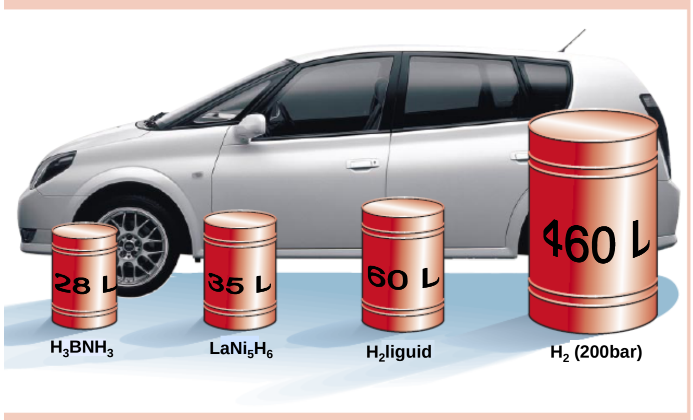
Porous Cage/Channel Structures



Molecular Encapsulation Frameworks

Major issues in hydrogen storage materials studies:

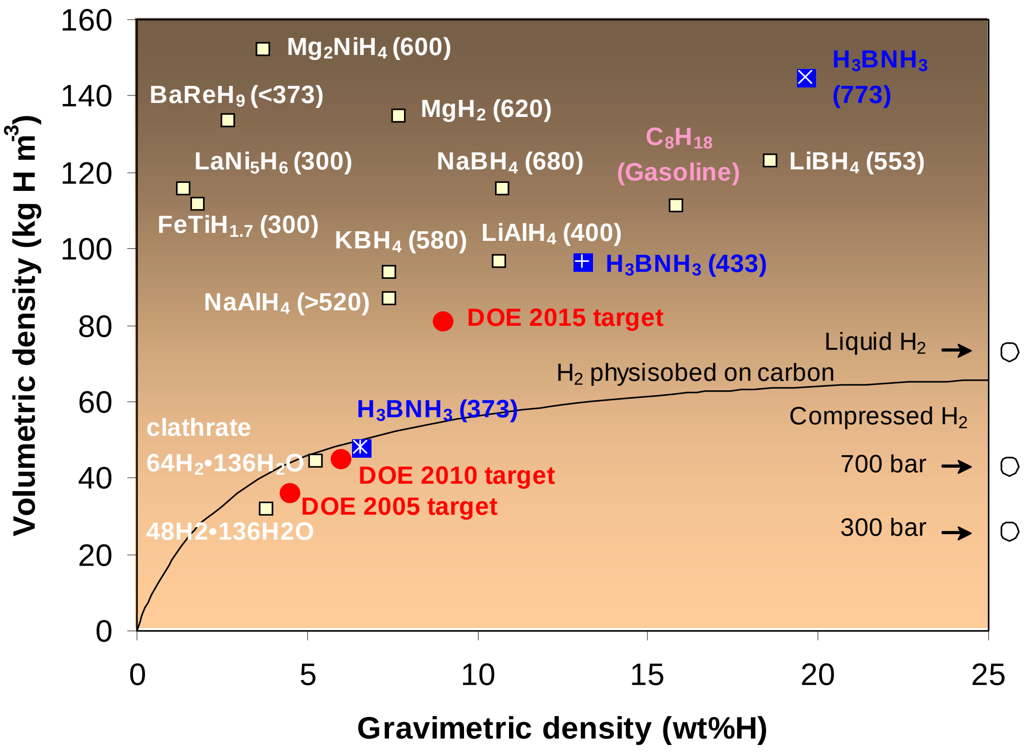
hydrogen density and rehydrogenation

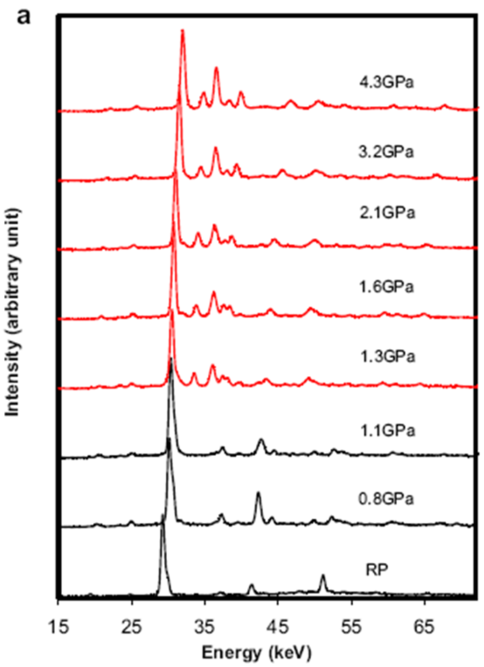


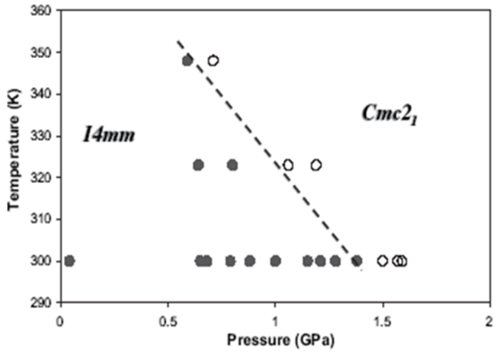
Hydrogen as on-board energy source:

4 kg H_2 / 400 km

Ammonia Borane NH_3BH_3 is a high hydrogen density material with a high release rate, however, rehydrogenation is difficult!





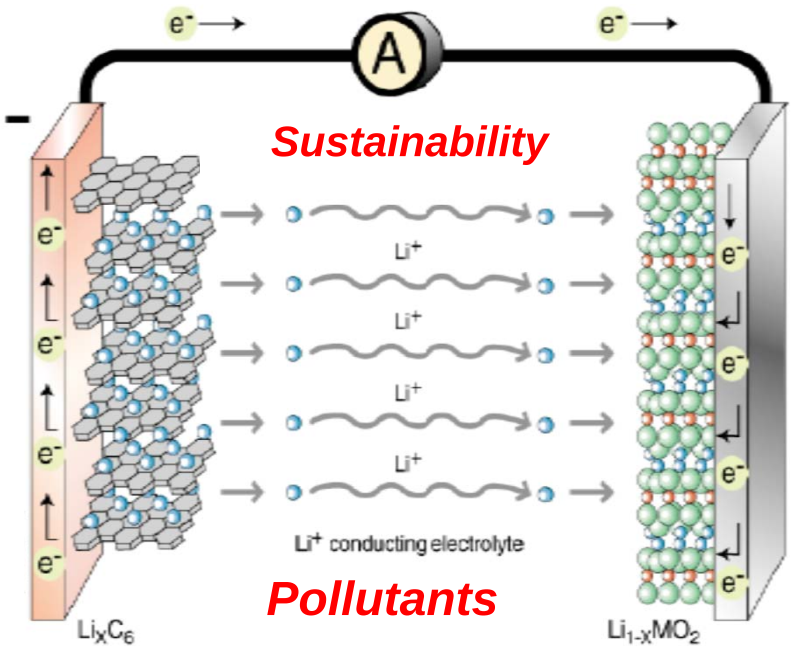


Can high pressure aid Rehydrogention of

Ammonia Borane

Low energy density

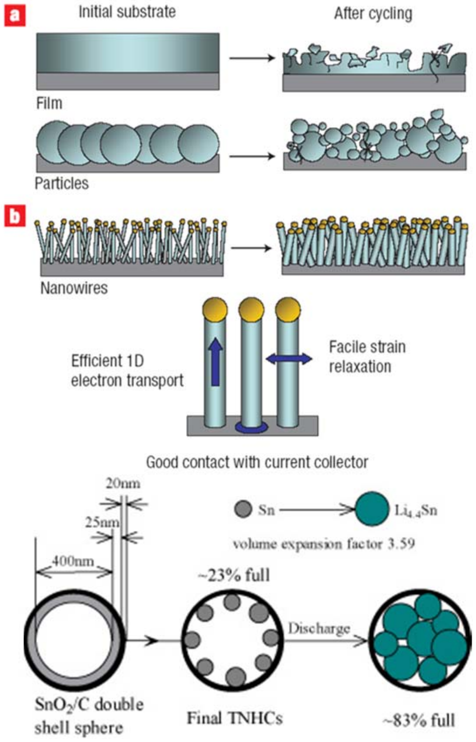
Sustainability

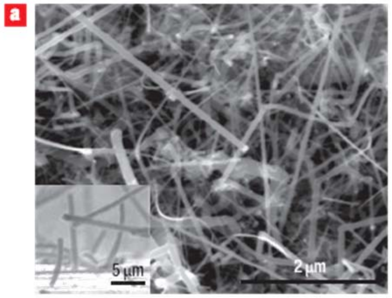


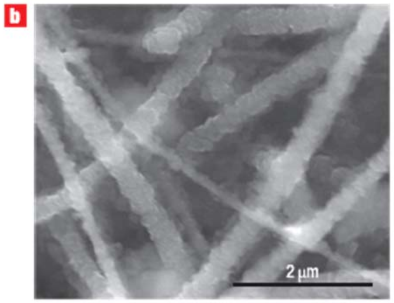
Pollutants

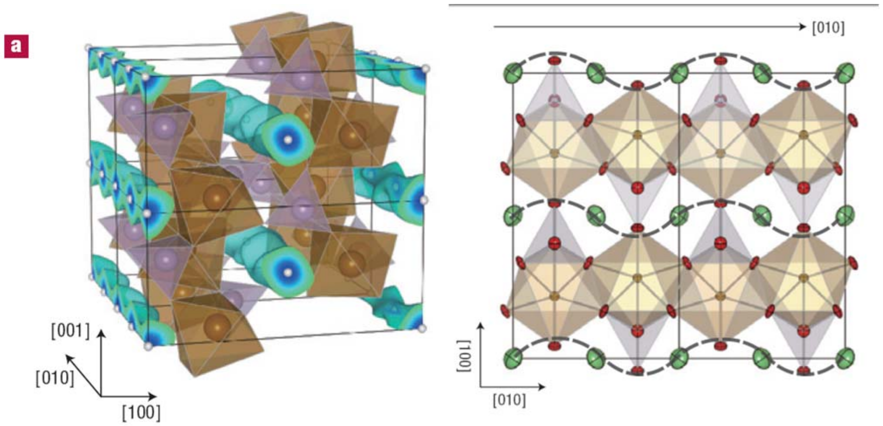
Heavy & Expensive

Problems!!!

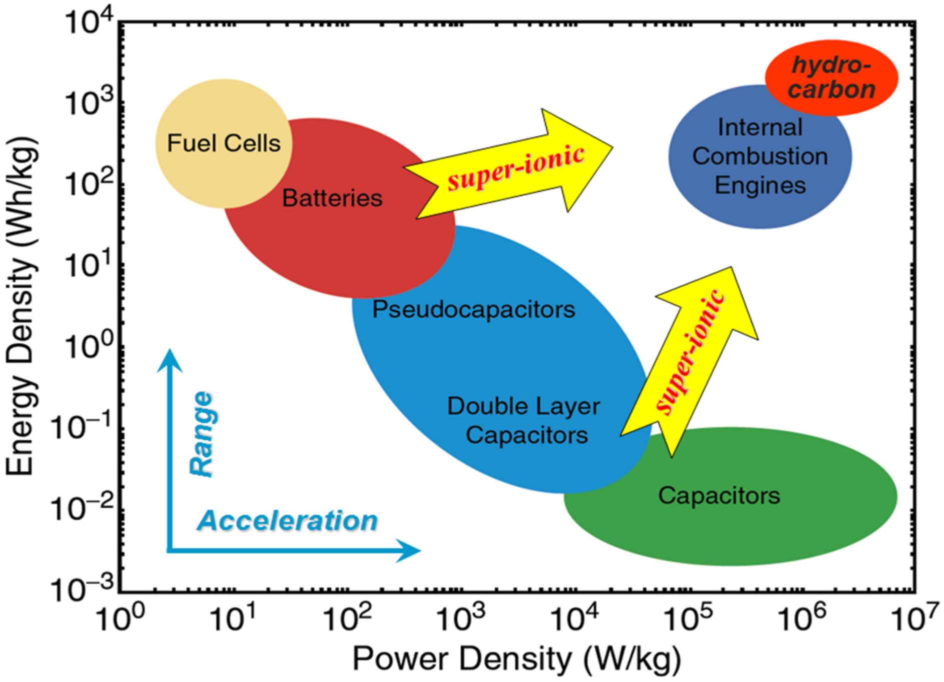


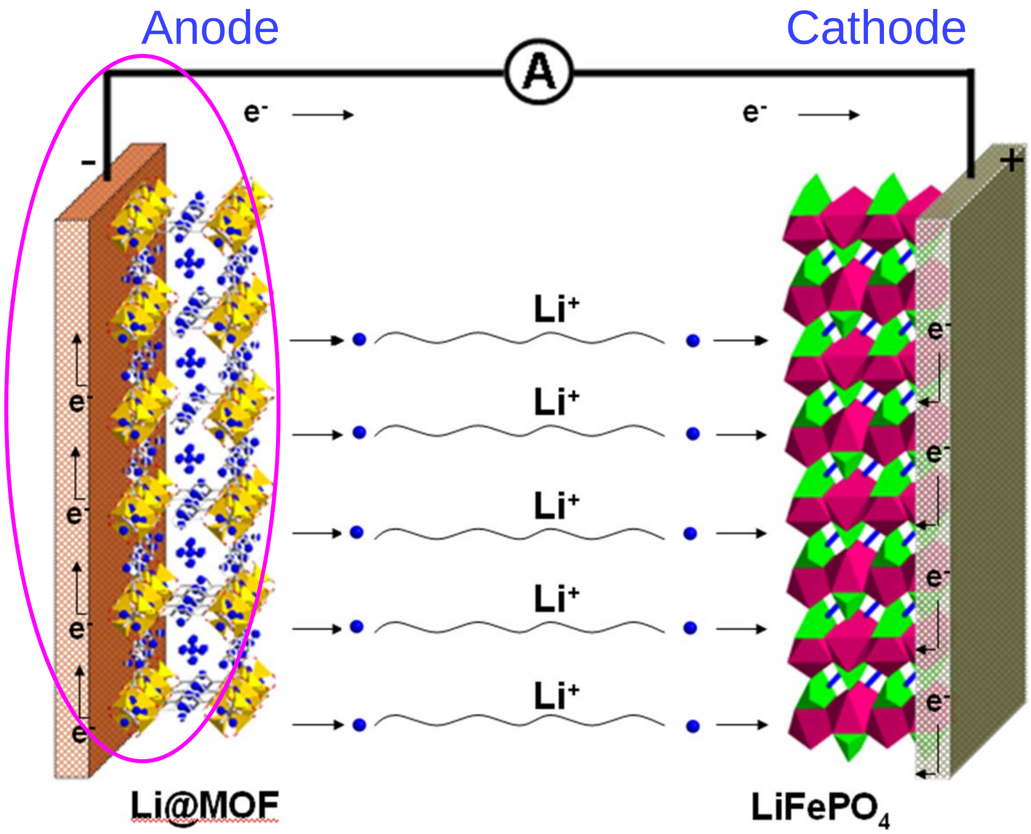




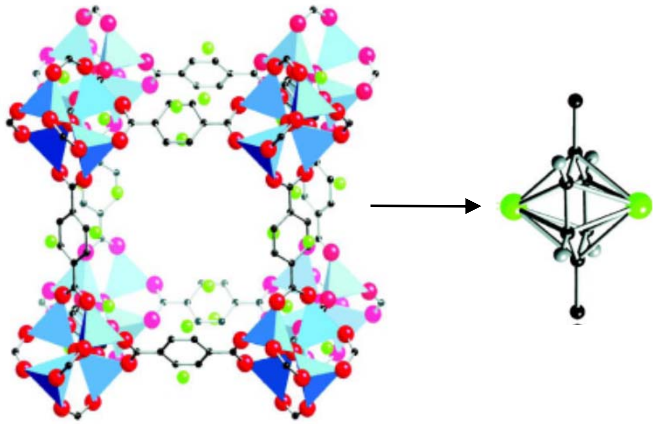


The molecular encapsulation and pressurizing effects has inspired us to investigate high lithium storage possibility. Conducting MOFs, zeolites, and clathrates offer a route to design the nano-architecture of electrode with high specific energy (high Li density!) .



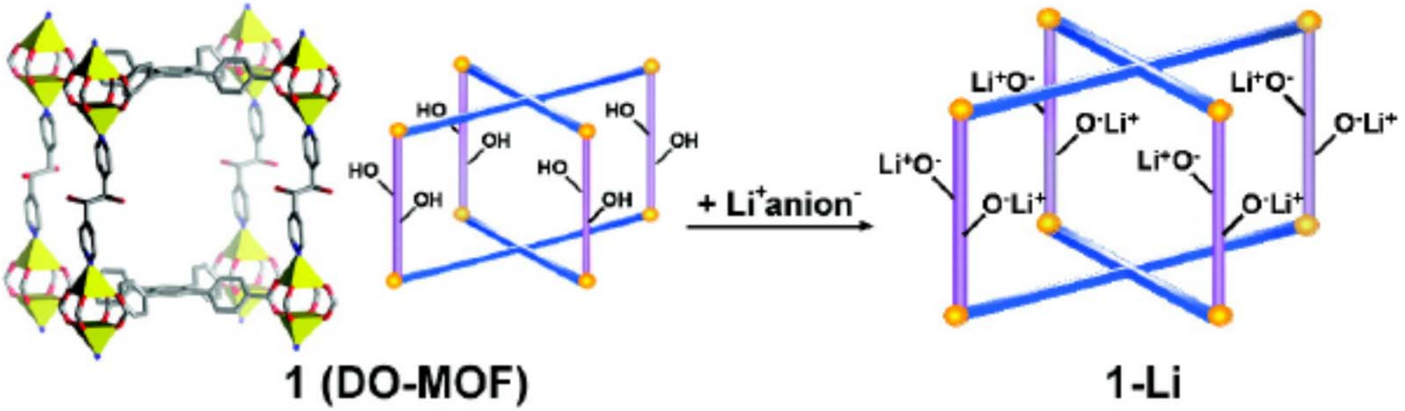


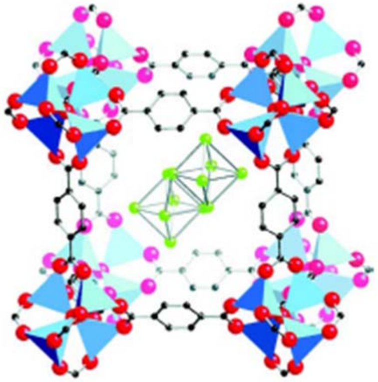
theoretical simulation



Li(+0.9e)-decorated MOF-5

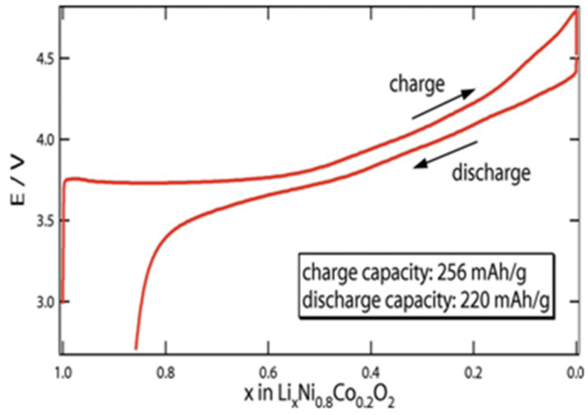
Alkoxide approach as a means of incorporating Li storage



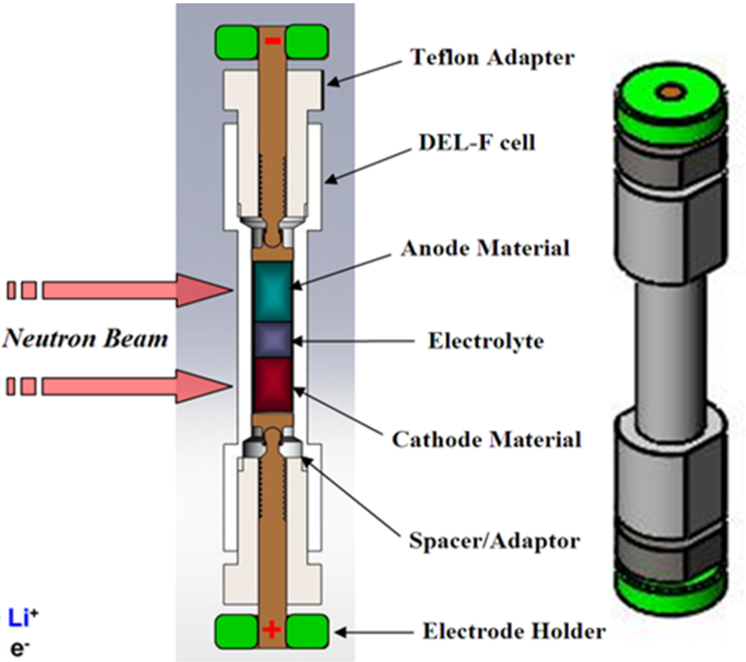


MOF-5 with Li_{12} cluster in cage

nSEC : Integrated Neutron Scattering, Electrochemistry, and Calorimetry Studies



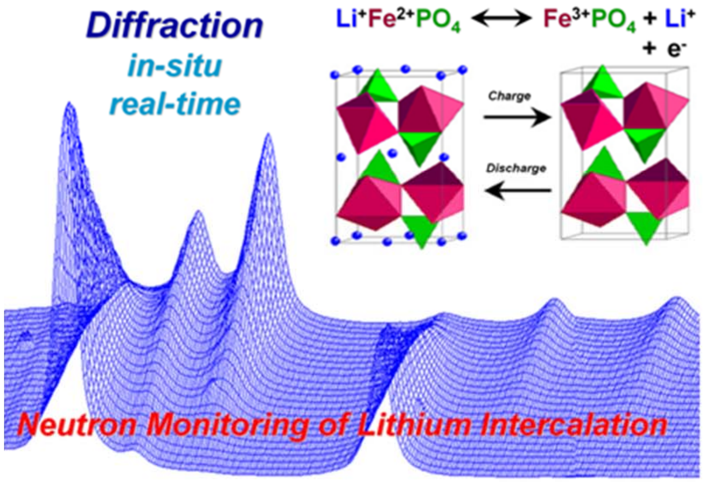
charge/discharge cycles



Potentiostat

Thermal Analyzer
DTA, DSC

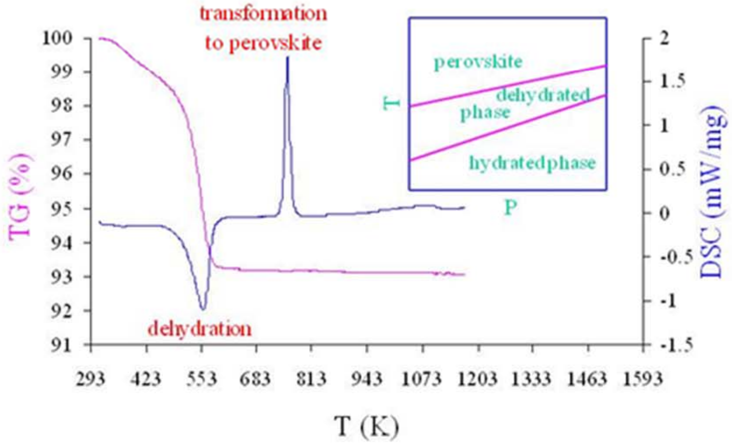
Temperature
Controller



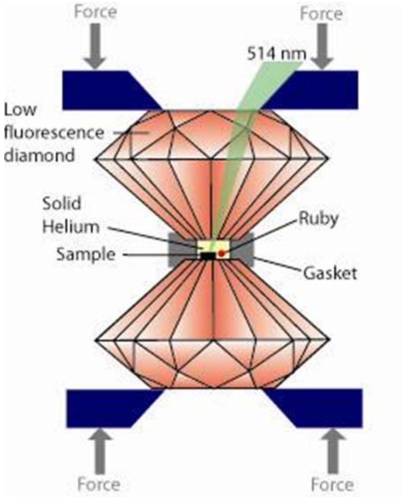
Diffraction
in-situ
real-time

$Li^{+}Fe^{2+}PO_4 \leftrightarrow Fe^{3+}PO_4 + Li^{+} + e^{-}$

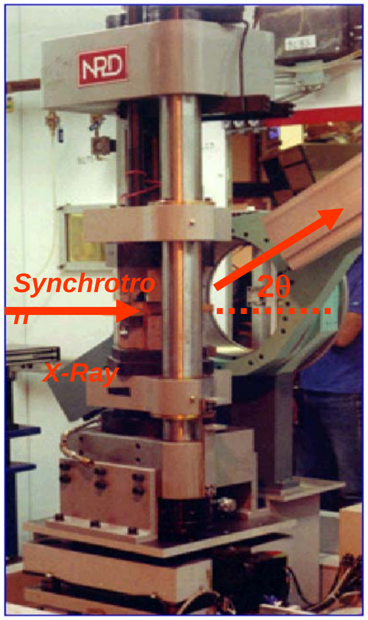
Neutron Monitoring of Lithium Intercalation



Neutron can "see" the movement of lithium ions and detect fast ionic transporting channels in the crystal structure, then provide guides on crystal engineering and synthetic chemistry!

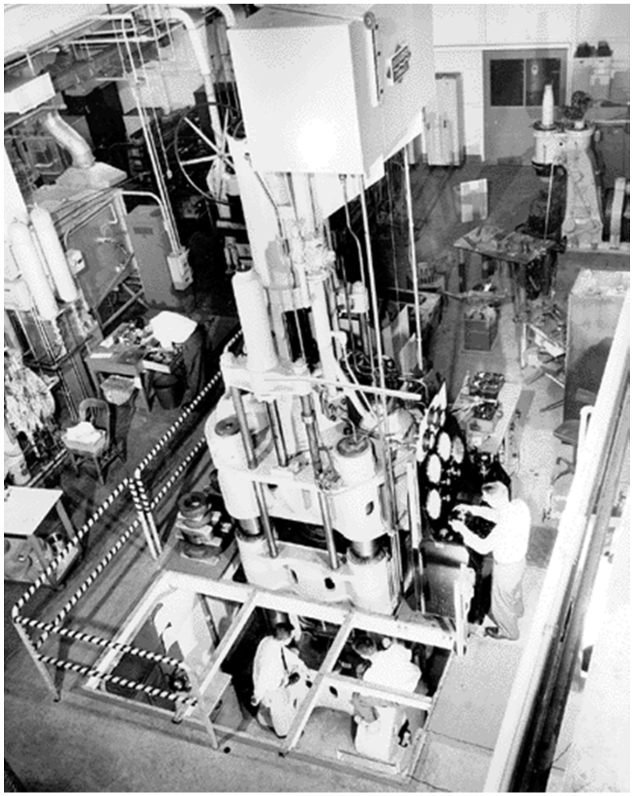


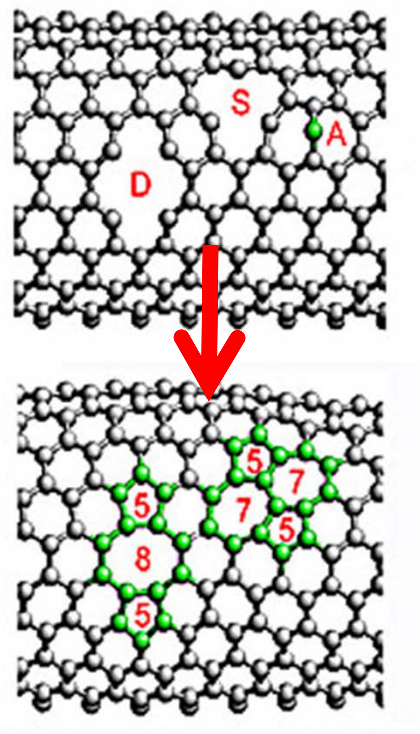
Diamond Anvil Cell



Multi-Anvil

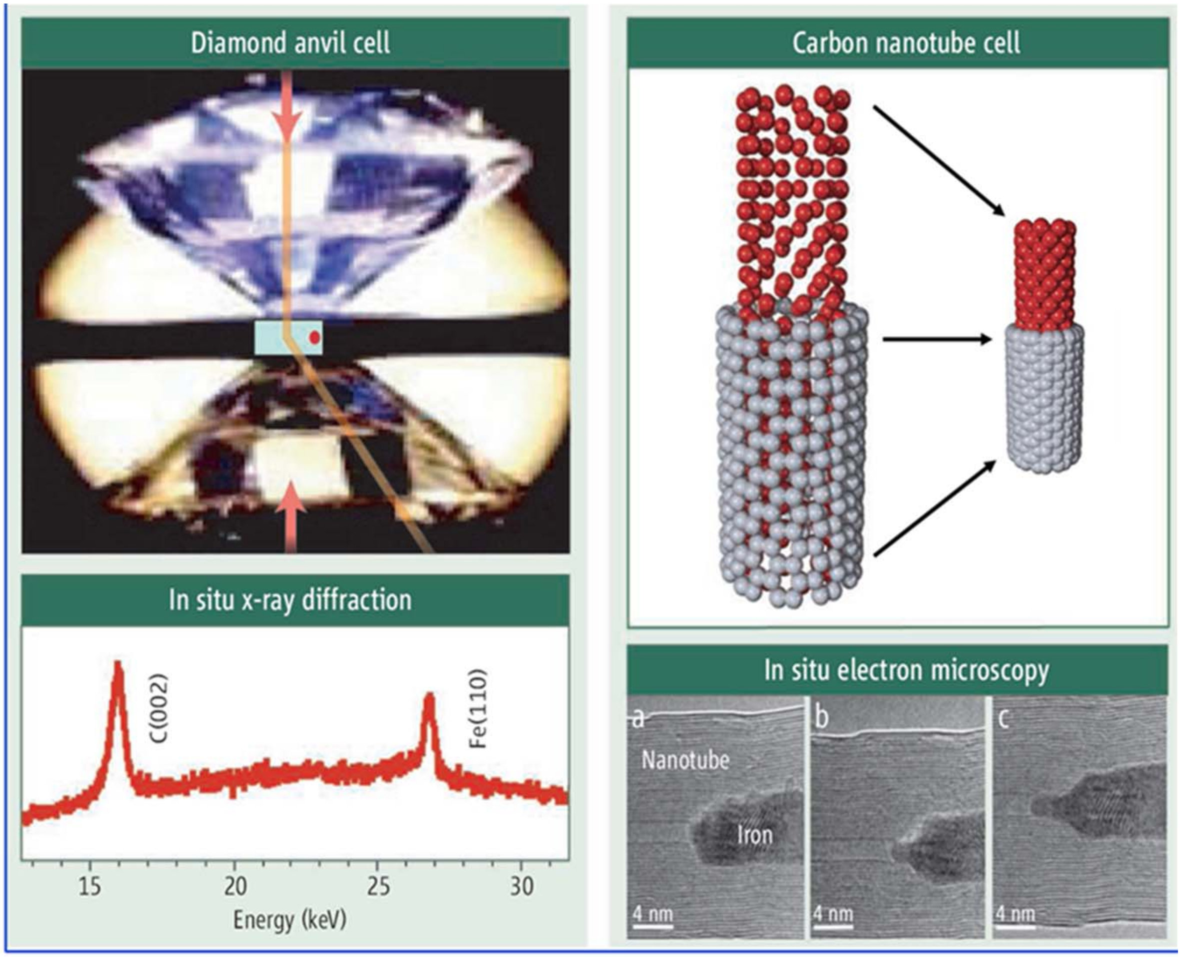
Toroidal Anvil

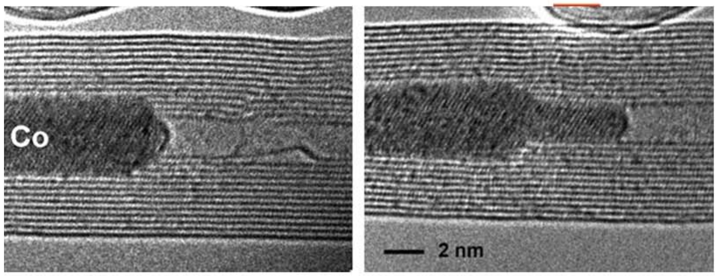


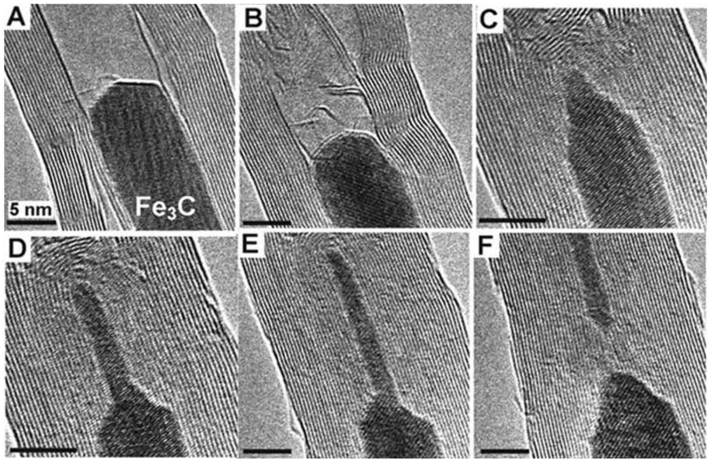


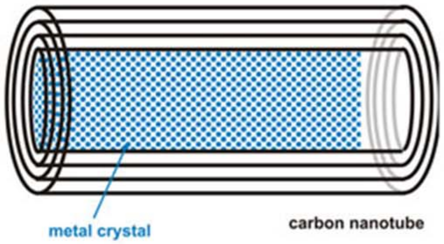
High-Pressure Microscopy

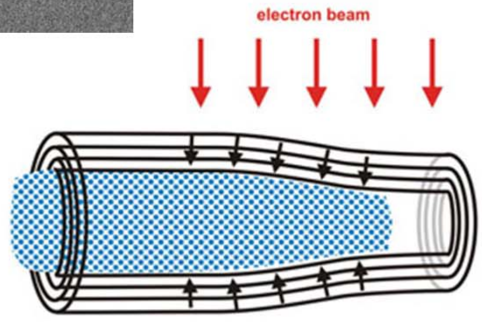
nanotube as a high-P squeezer!





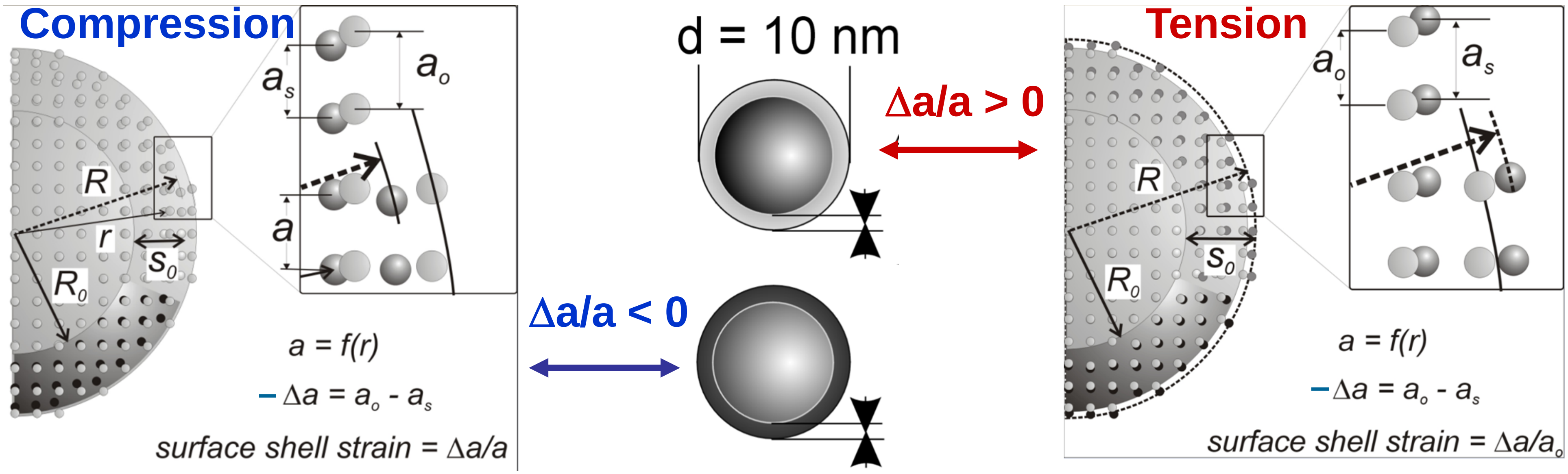






Initial enhancement of bulk modulus observed for the nano-ceramics may result from the “pre-” **compressed** surface lattices in the **shell** volume of the nano- crystal grains;

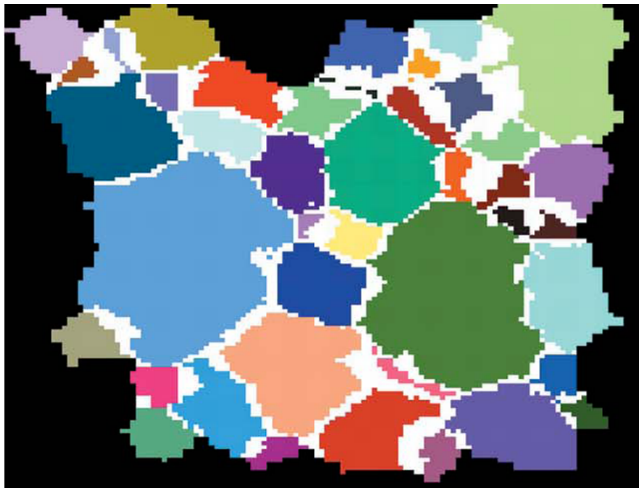
The high pressure induced work-weakening/cold-welding type of grain growth ***fuse*** surface shell with bulk cores, correspondingly the elastic modulus reduces/approaches the bulk values at high-pressures after P_c.

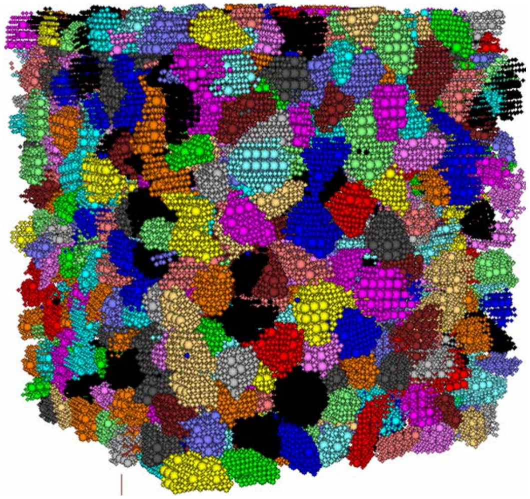


Initial reduction of bulk modulus observed for the nano-metals may result from “pre-” **expanded** surface lattices in the **shell** volume of the nano- crystal grains;

High pressure induced work-hardening after the bulk yield reflects continuous densification of the surface shell while bulk core also experience compression.

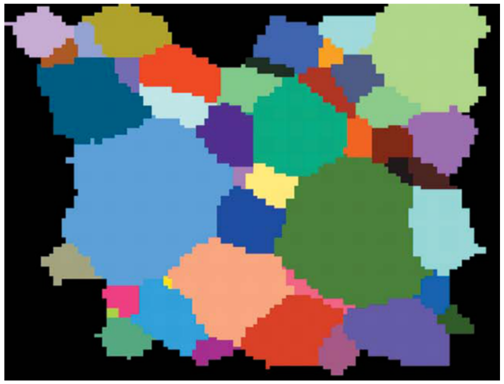
Macro- *vs* micro- *under pressures*





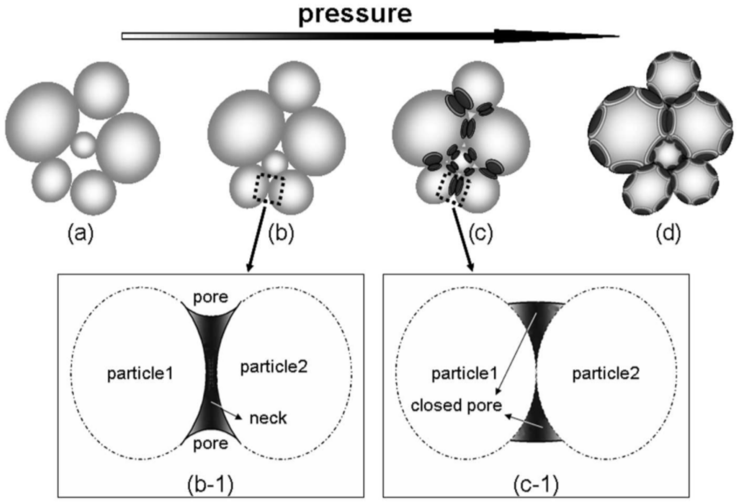
Powder Compaction

(*micro-strain*)

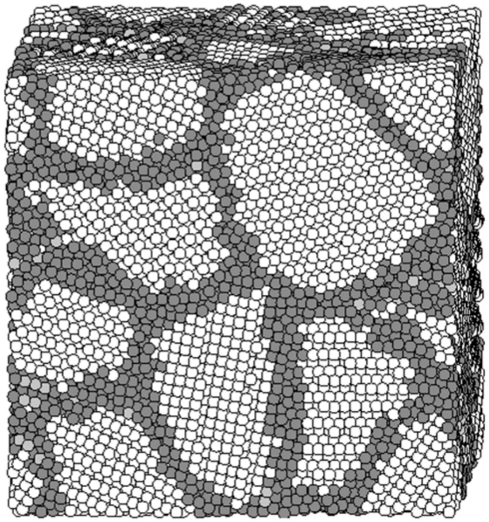


Deviatoric Stress

(*macro-strain*)



***grain-to-grain* contact stress concentration**



(a), relaxed lattice

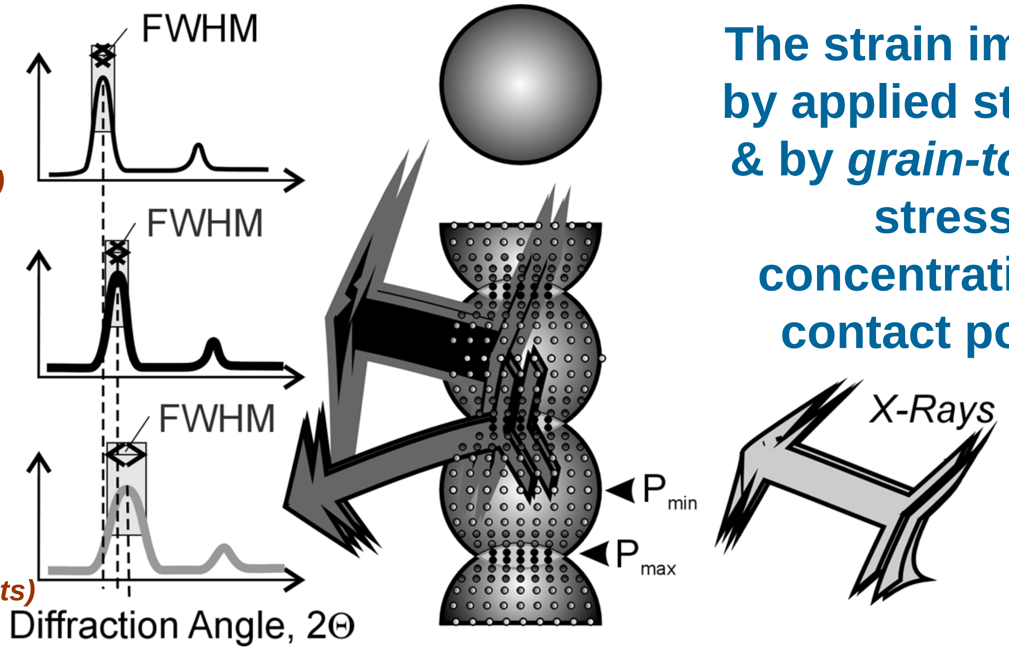
(no stress applied on the "infinite" atomic lattices)

(b), macro-strains

(stress field applied to the overall sample)

(c), micro-strains

(stress concentration due to grain-to-grain contacts)

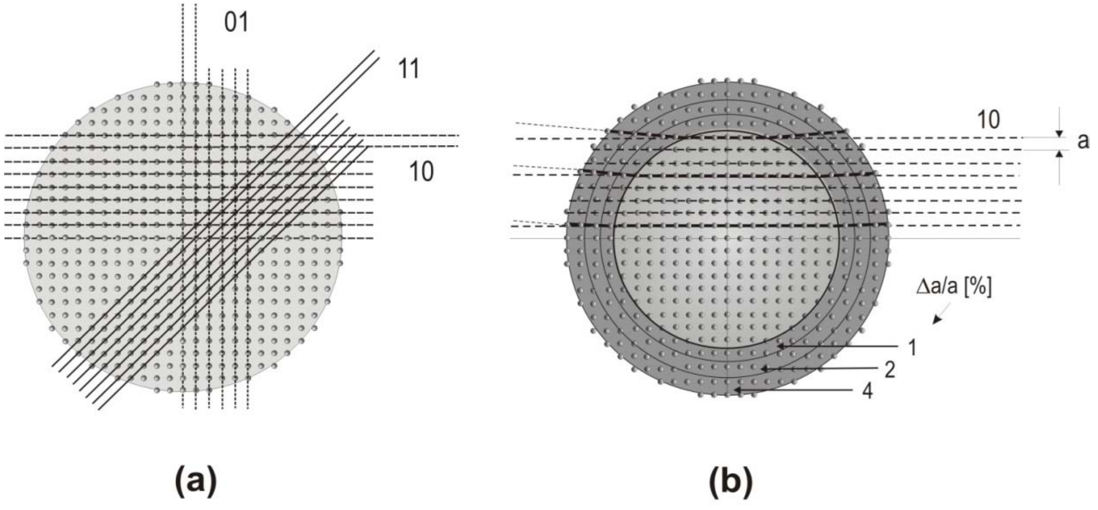


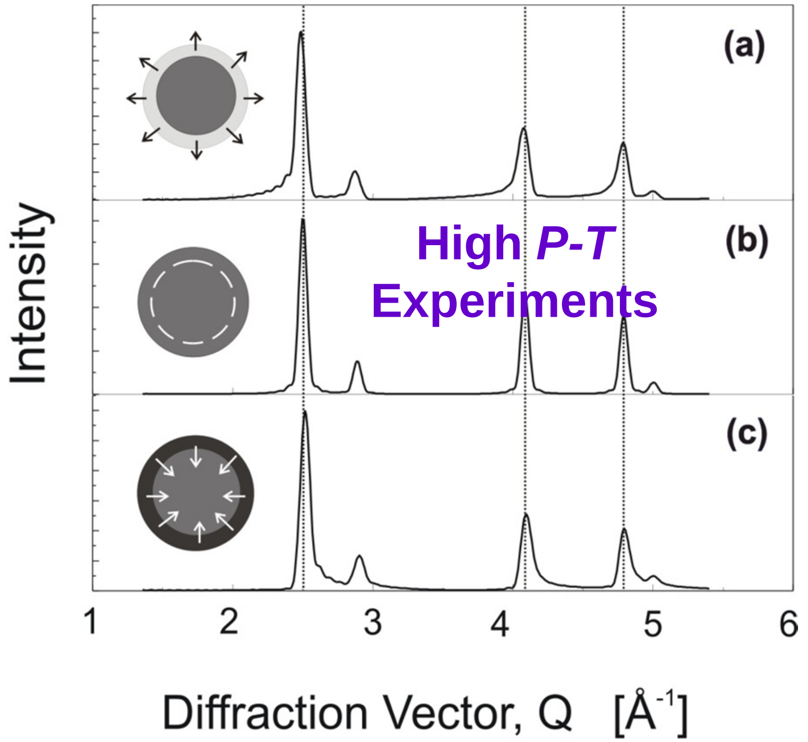
The strain imposed by applied stresses & by *grain-to-grain* stress concentration at contact points

nano-crystal

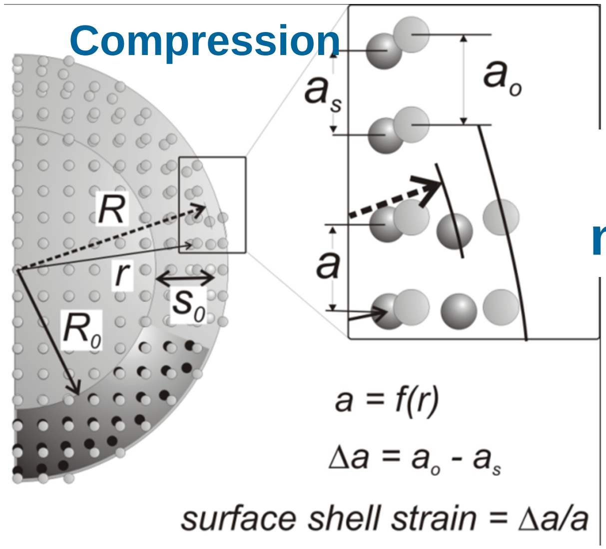
Uniform Core and Strained Surface

***Palosz* Model**





High *P-T* Experiments



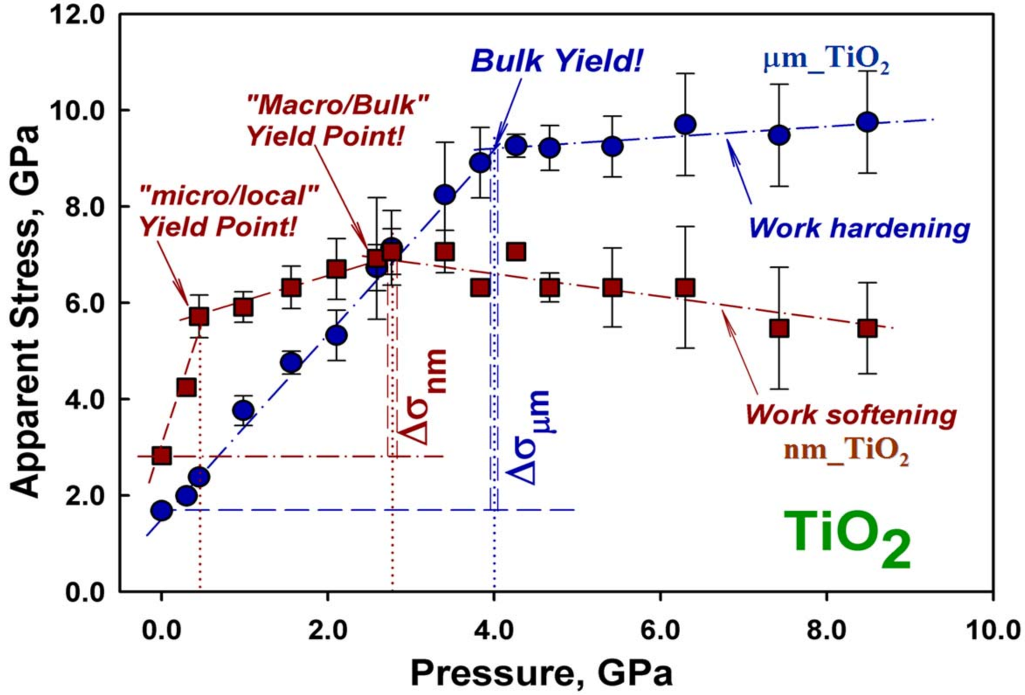
$a = f(r)$

$\Delta a = a_o - a_s$

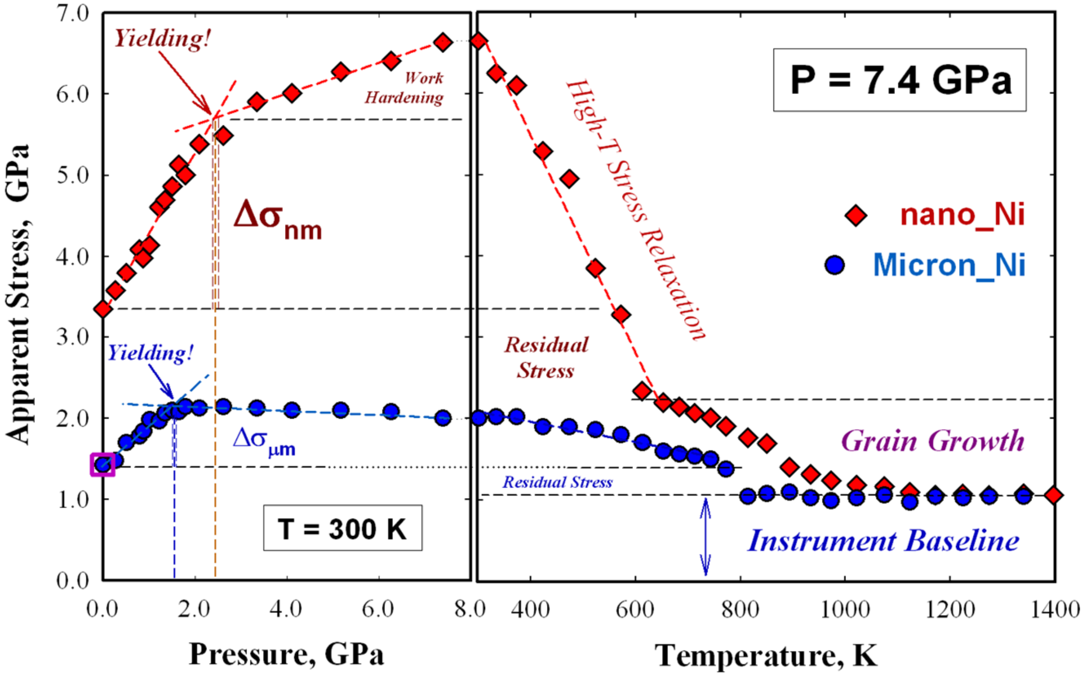
surface shell strain = $\Delta a/a$

Ceramic nano-TiO_2

$$a_s < a_o$$



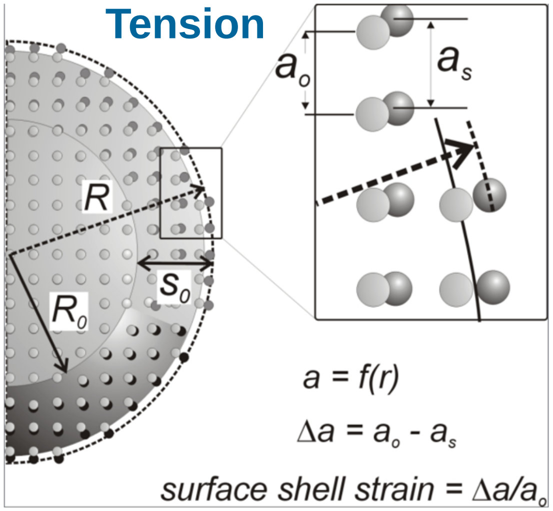
Ceramic nano-TiO_2 with compressed shell shows work-weakening under stress (P)



Metal nano-Ni with tensile shell shows work-hardening under stress (P)

Metal nano-Ni

$$a_s > a_o$$



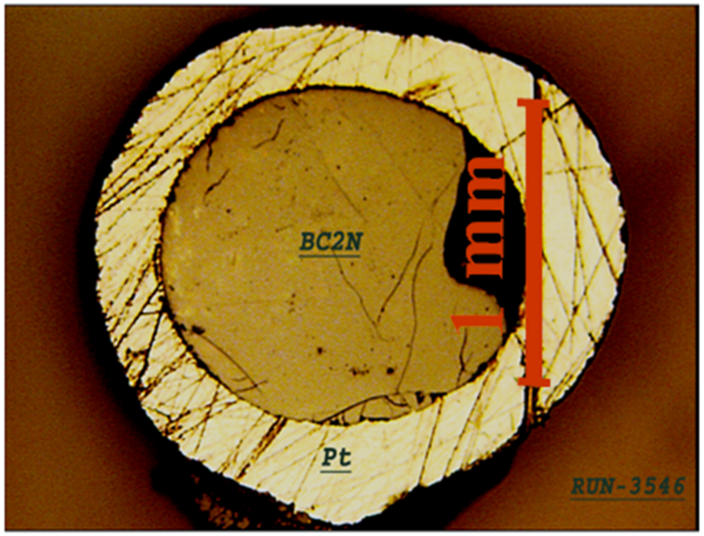
$a = f(r)$

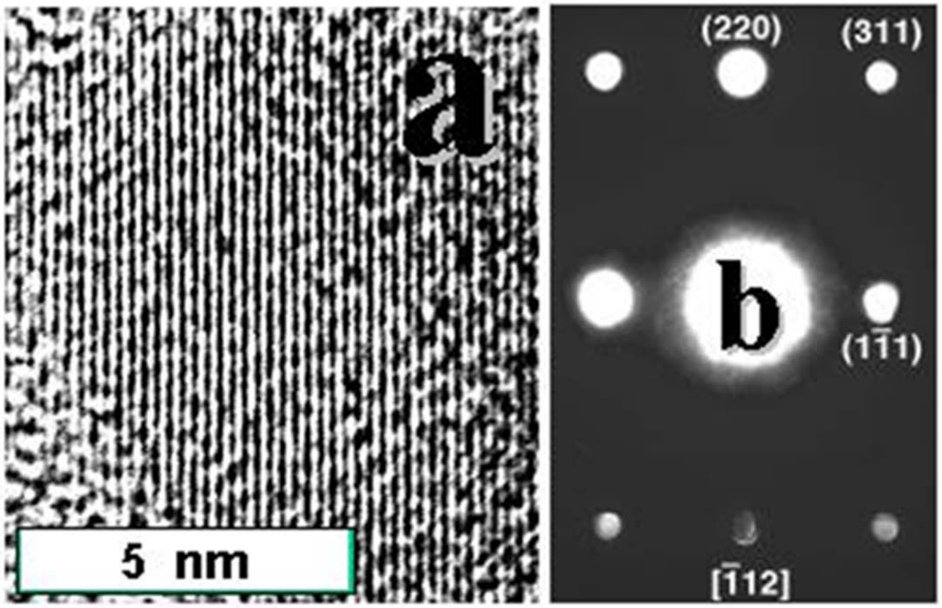
$\Delta a = a_o - a_s$

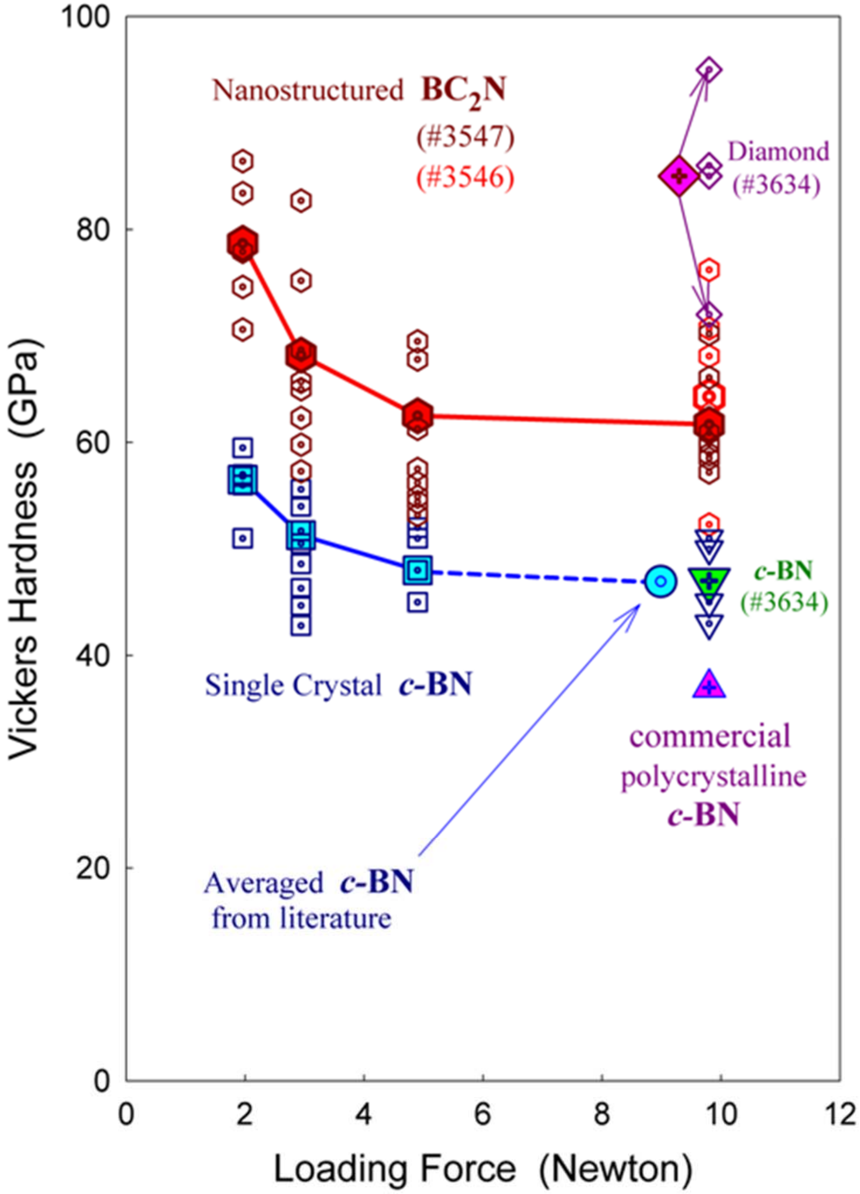
surface shell strain = $\Delta a/a_o$

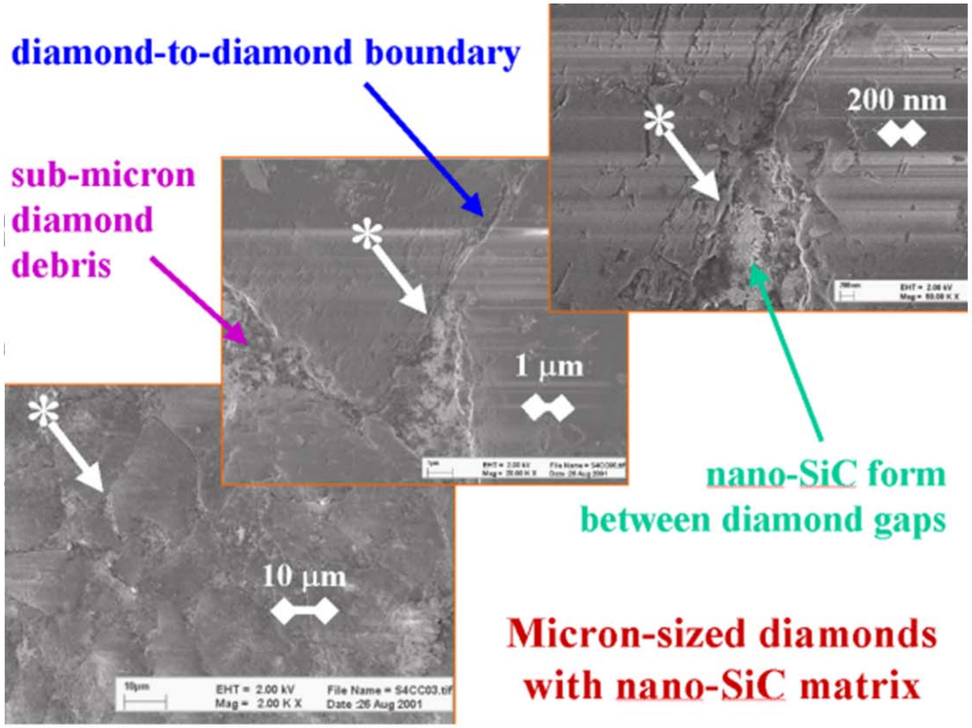
Characterization of the B-C-N sample

Vickers hardness measurement of BC_2N







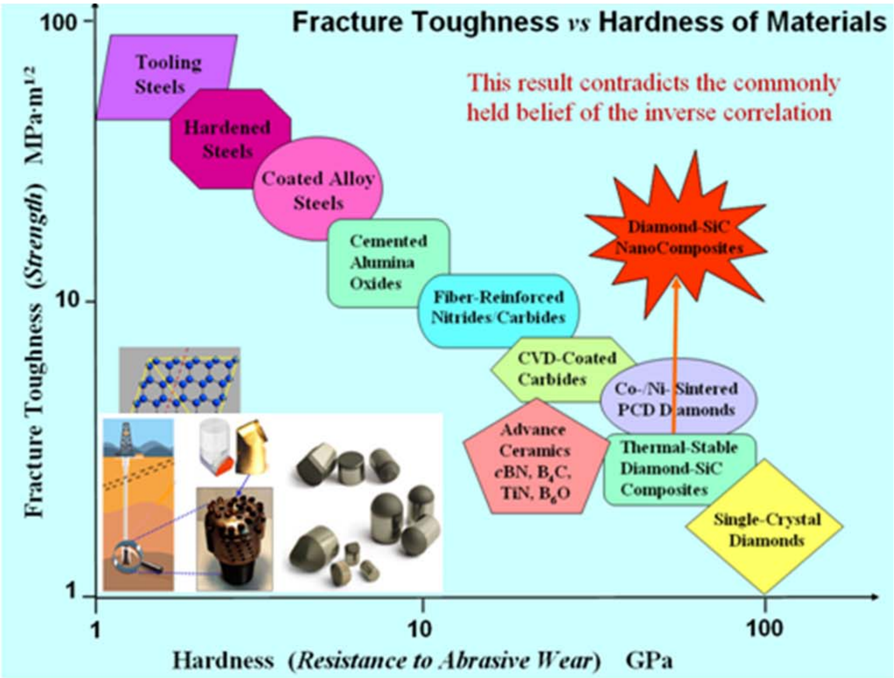


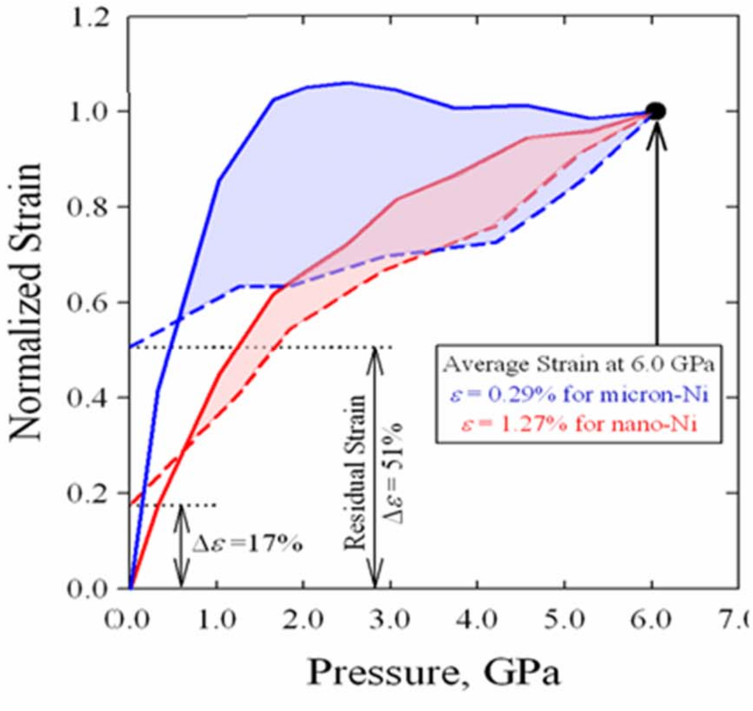
diamond-to-diamond boundary

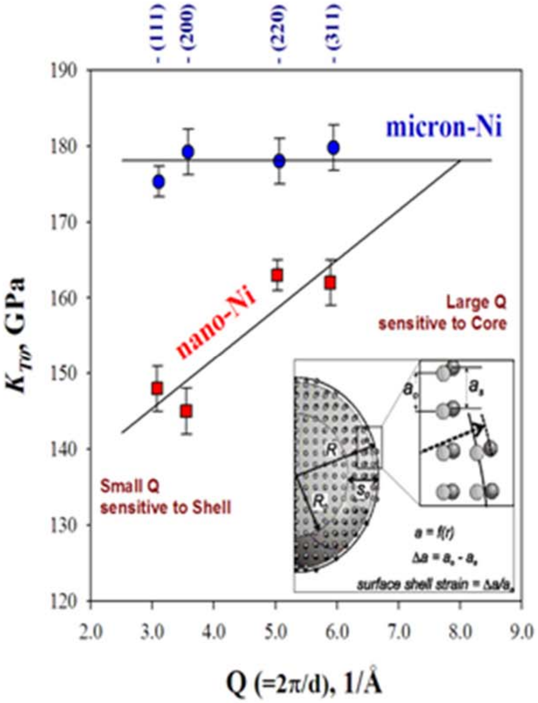
sub-micron diamond debris

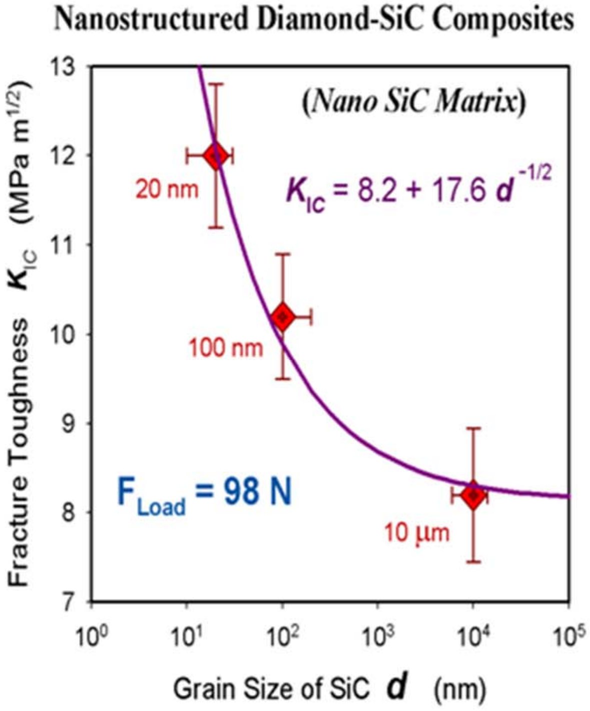
nano-SiC form between diamond gaps

Micron-sized diamonds with nano-SiC matrix

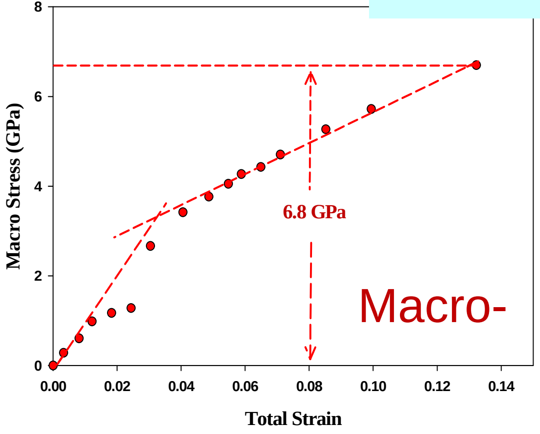


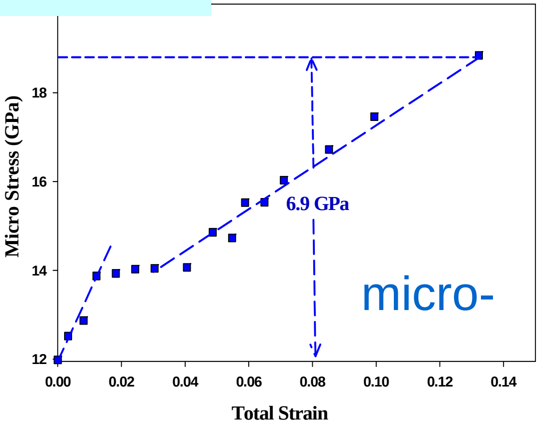




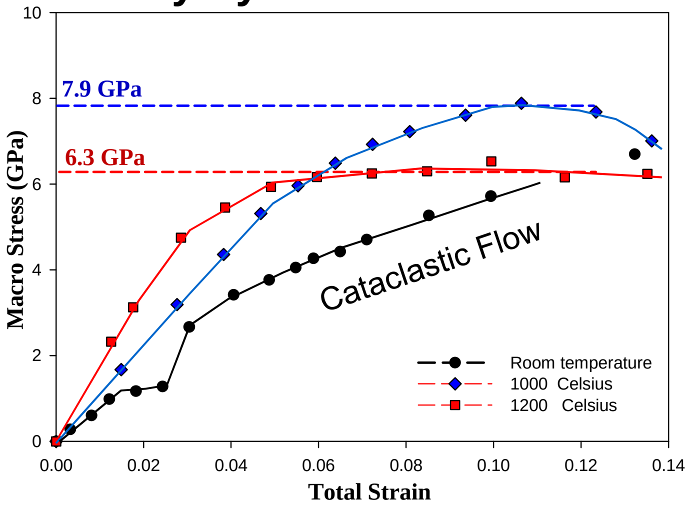


P = 4 GPa,   T = 300 K

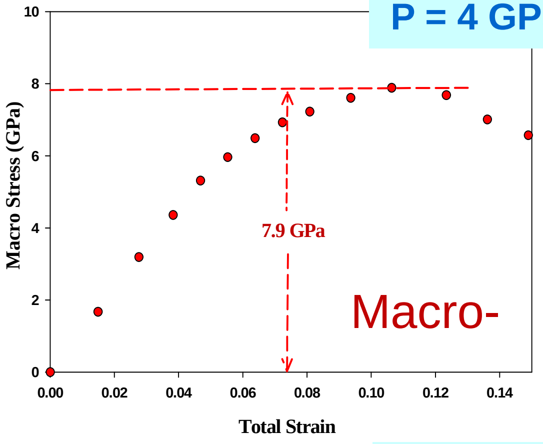


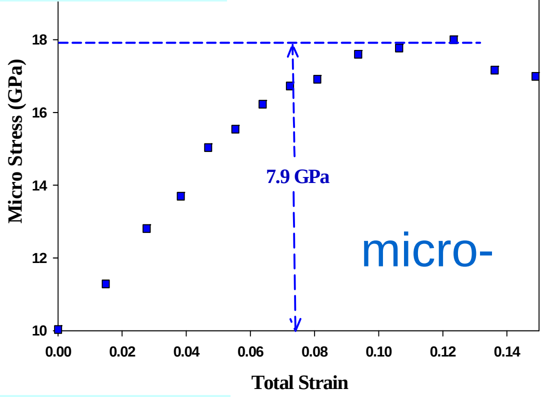


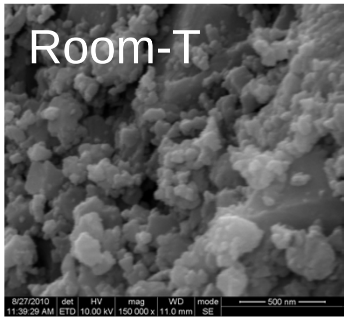
Polycrystalline Diamonds

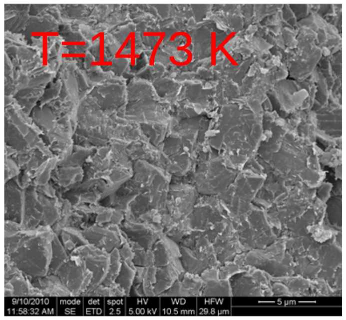


P = 4 GPa,   T = 1273 K

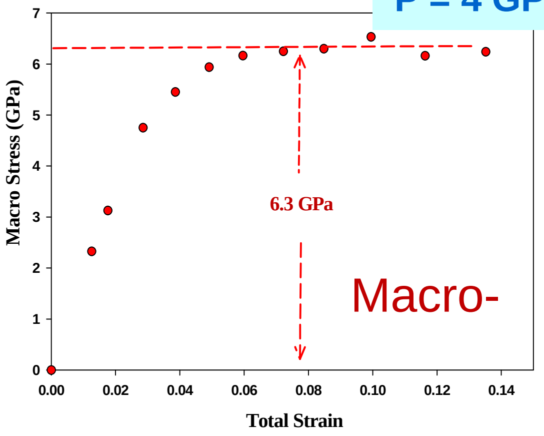


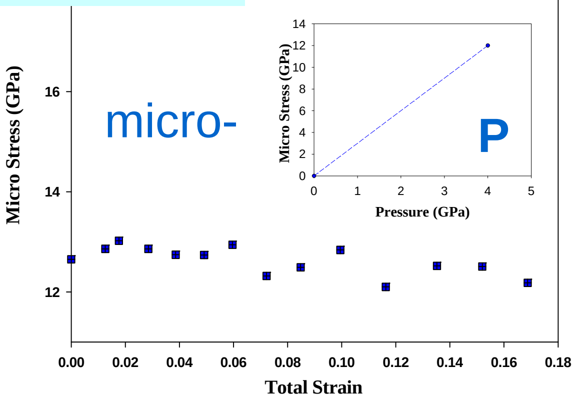


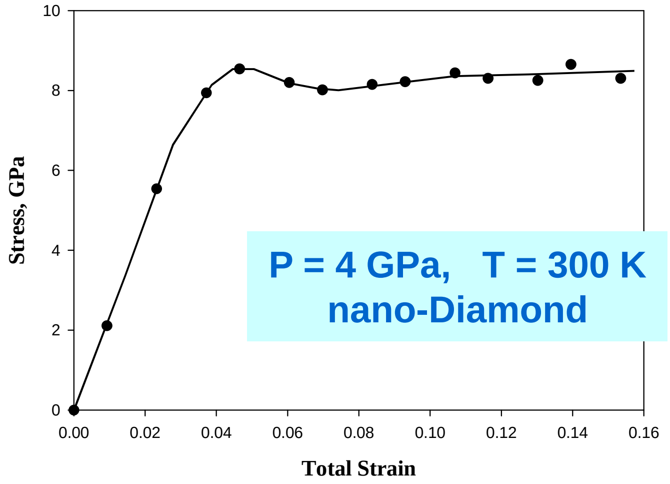




P = 4 GPa,   T = 1473 K

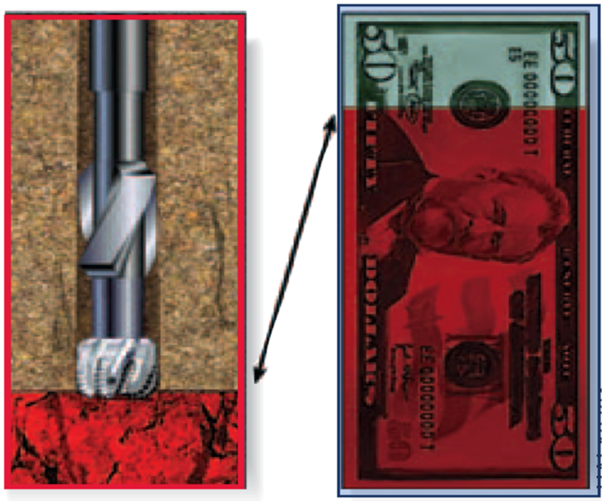






P = 4 GPa,   T = 300 K
nano-Diamond

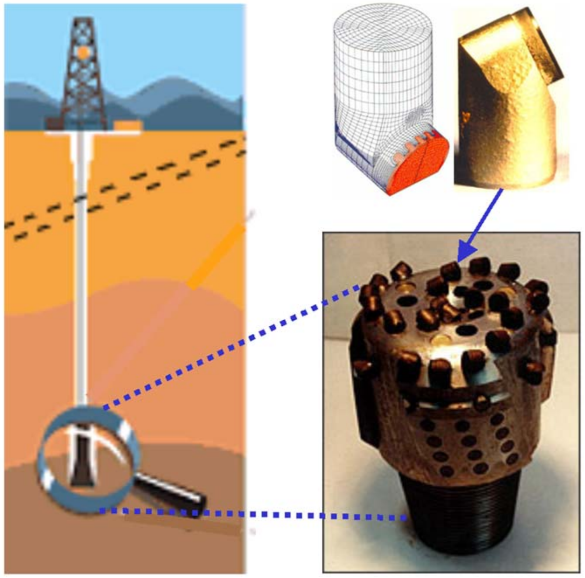
Time Consuming
Labor Intensive
High Risk

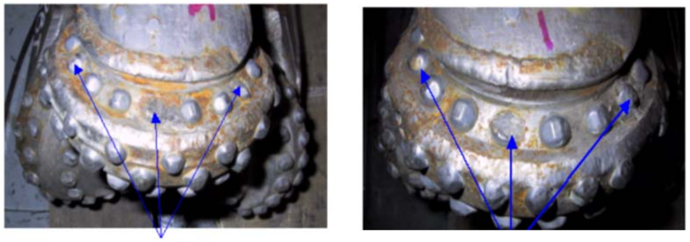


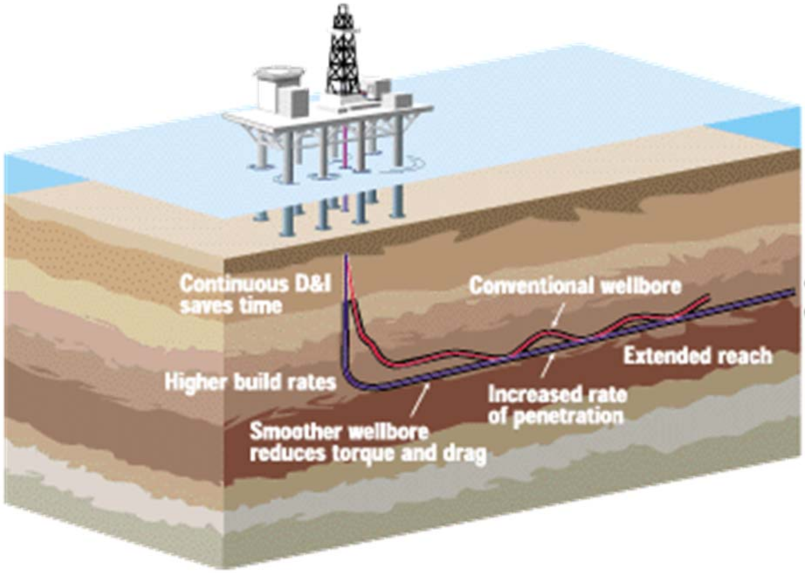
20% OF FOOTAGE

80% OF BUDGET

Harder & Tougher Drill-Bit

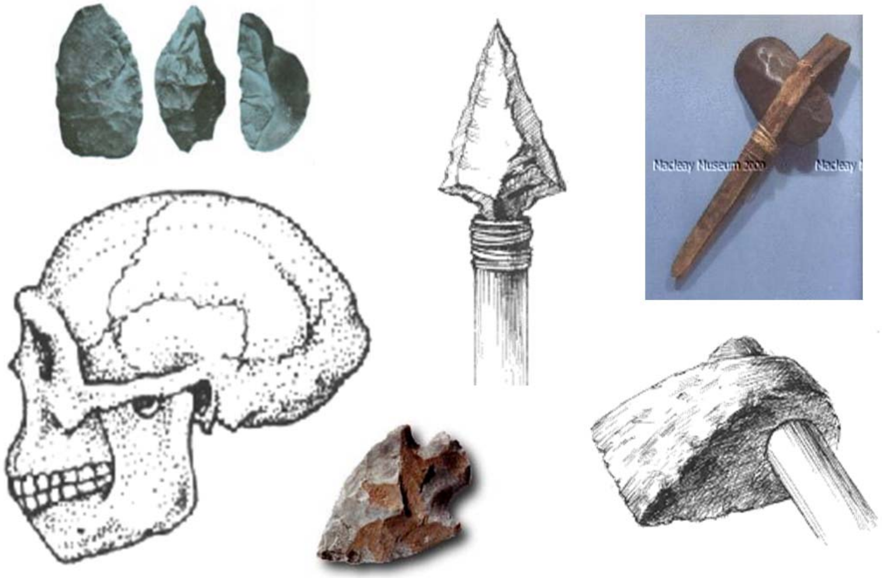


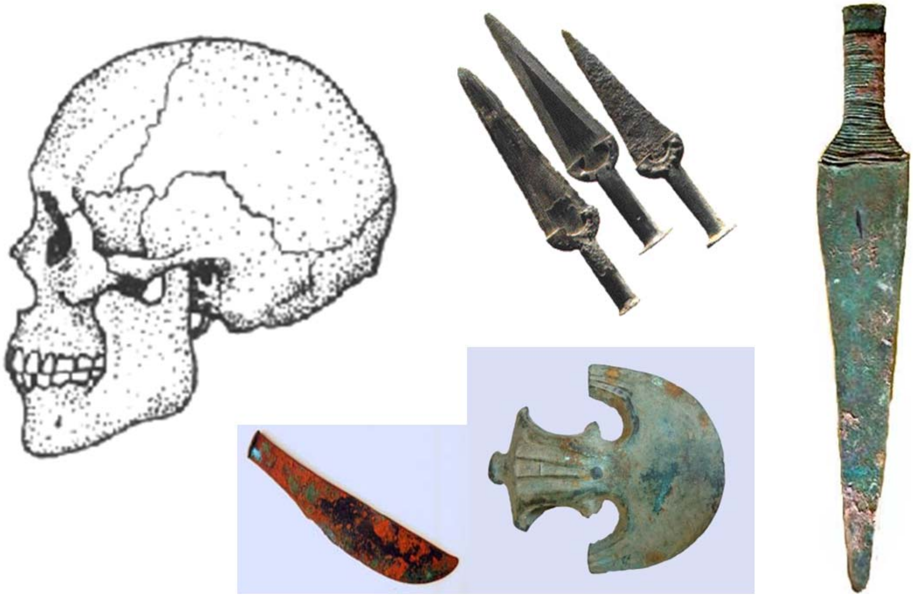




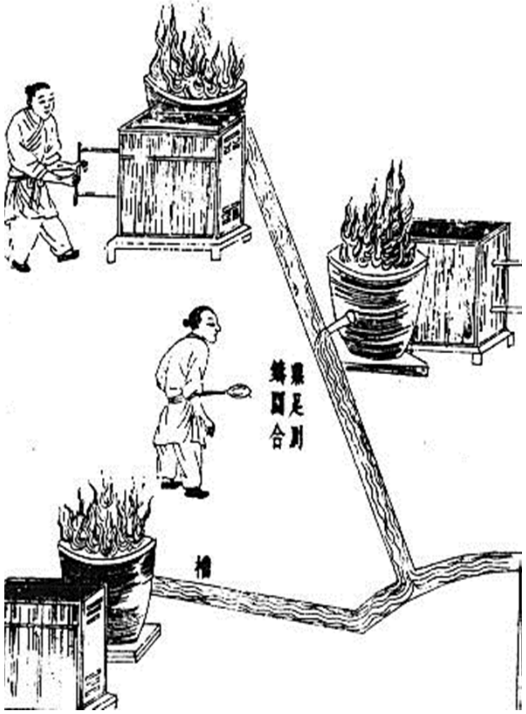
Human Evolution from Stone Age to Bronze Age

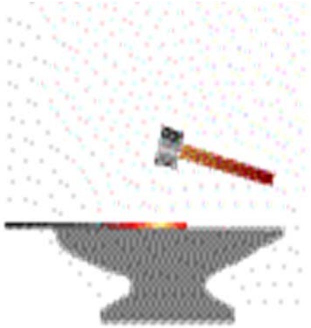
A History of Pursuing Harder & Tougher Tools

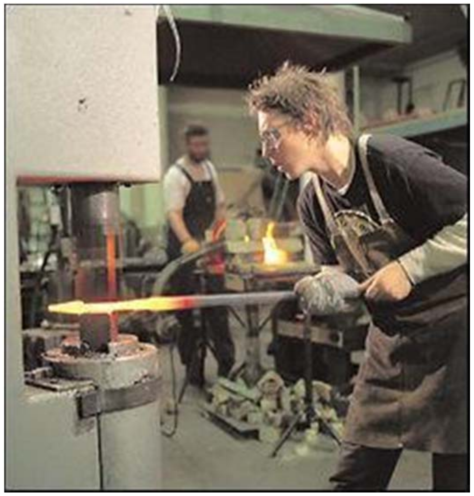


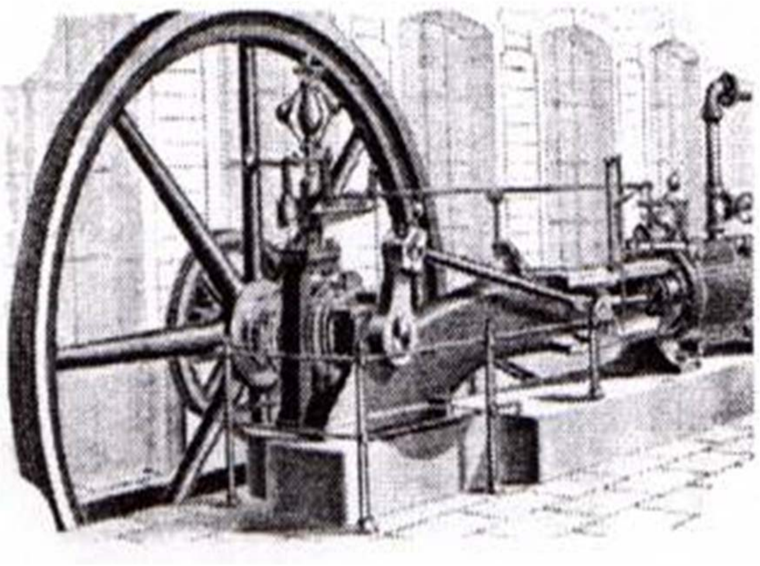


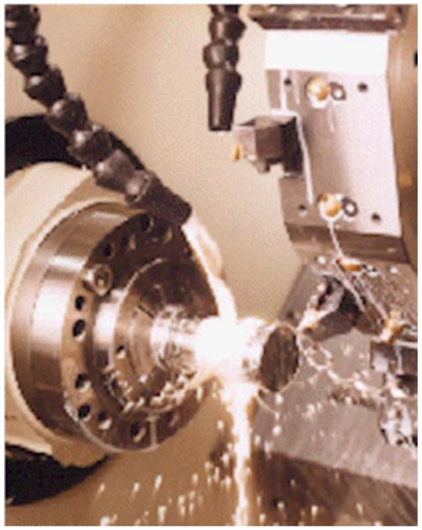
High-Pressure and High-Temperature Forged
Agriculture to Industrial Transformation

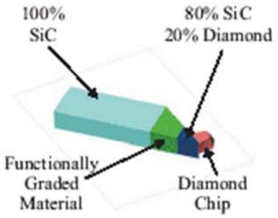




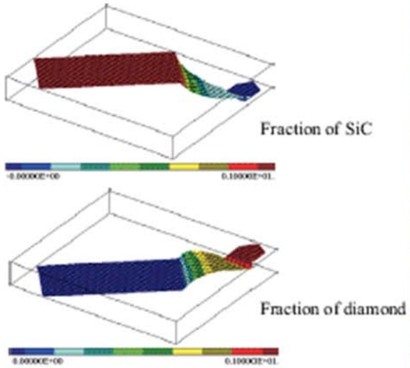








(a) Diamond cutter tool consists of several distinct material regions

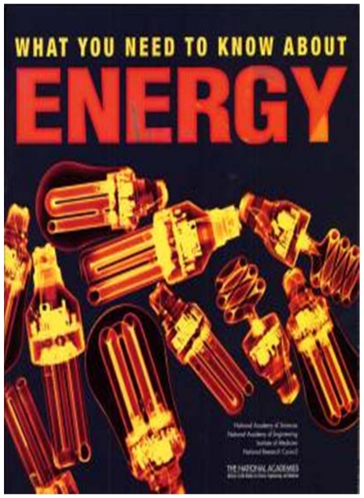


(b) Fractions of each material vary throughout the solid but always add to 1

Diamond/*c*BN Tools Are Widely Used in Modern Industries

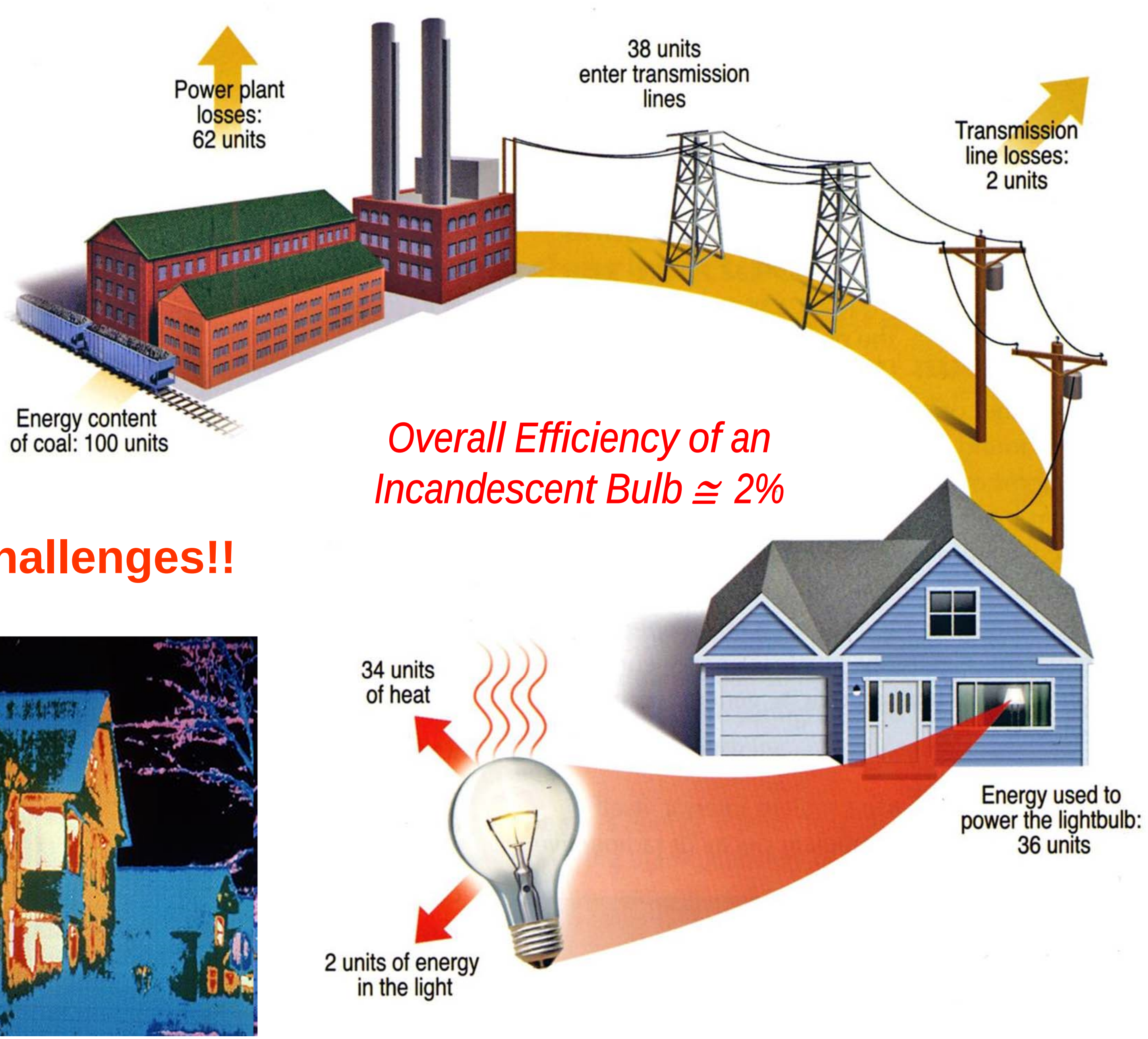
!! *Hardness, Toughness, Strength, & Thermal Stability* !!

The saved energy is the cleanest energy !



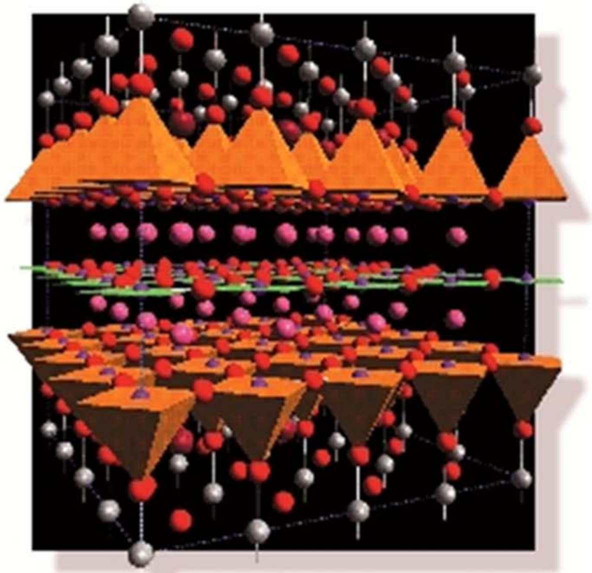
WHAT YOU NEED TO KNOW ABOUT

ENERGY



Overall Efficiency of an Incandescent Bulb ≃ 2%

Engineering Challenges!!

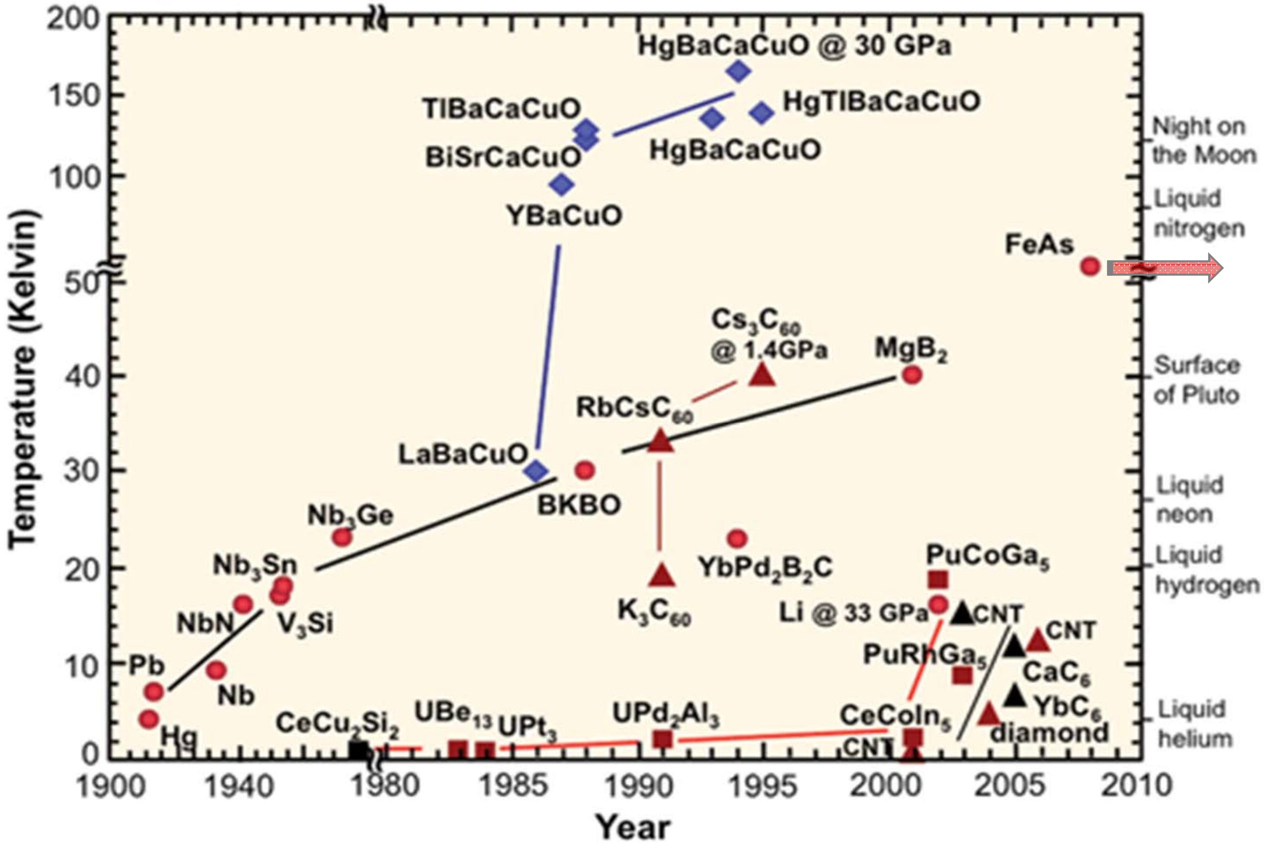


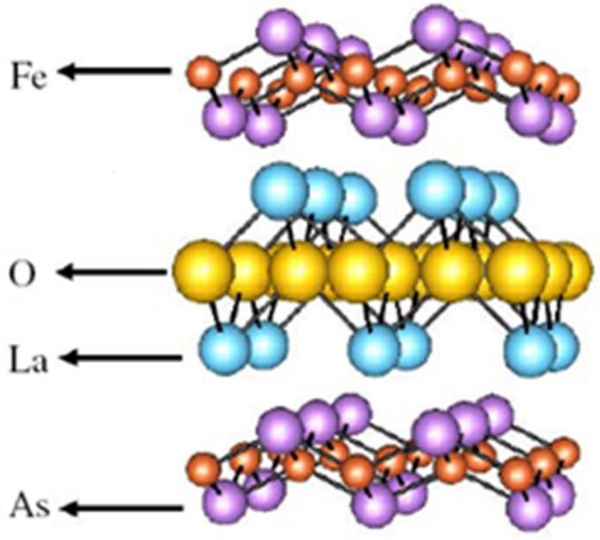
Crystal structure of high-T_c superconductor was first successfully determine by neutron diffraction (the classic ‘1-2-3’ $YBa2Cu3O7-x$ superconductor, published on *Nature* on 28 May 1987).

The neutron also first determined the antiferromagnetic interaction strength between copper electrons in the parent high-T_c La2CuO4.

Neutron study of HgBa2CuO4+d has revealed the structural basis for strong dependence of superconducting T_c on applied pressure.

Searching superconductors in P-T-X space

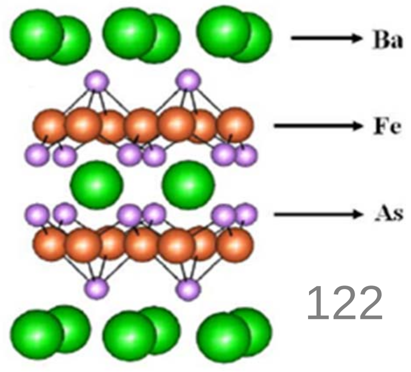




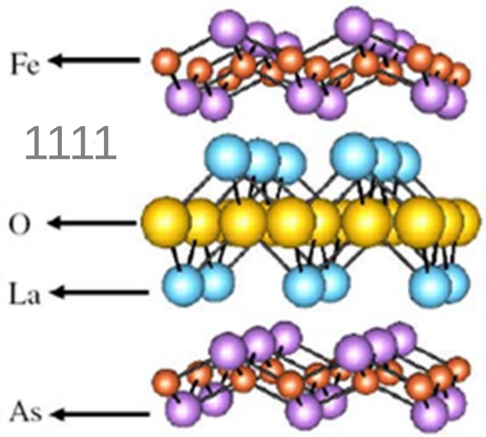
Sm based
iron SC
53 K

1111

Tetragonal
P4/nmm

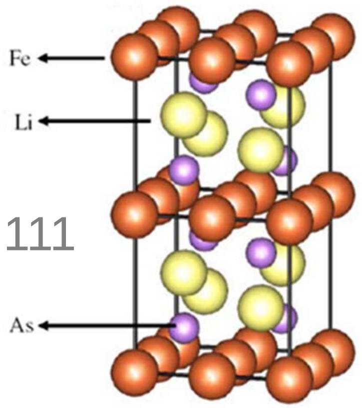


Tetragonal
I4/mmm

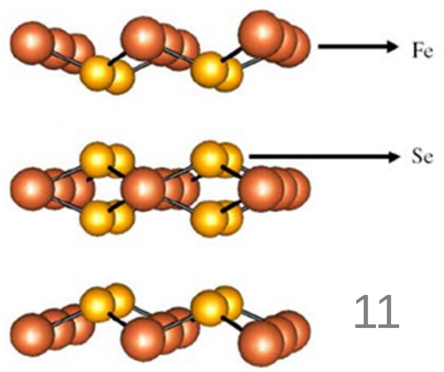


Aswathy *et al.*,
Supercond.Sci.Tech.
23, 073001 (2010)

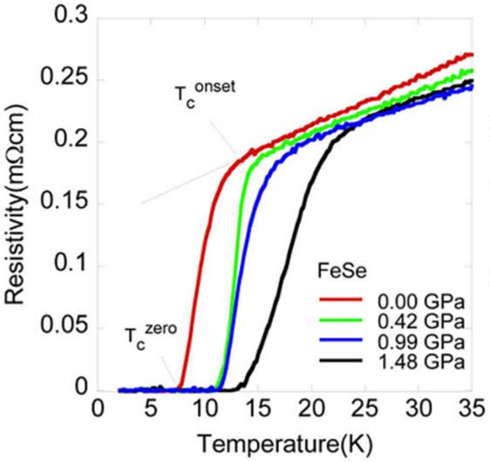
Tetragonal
P4/nmm

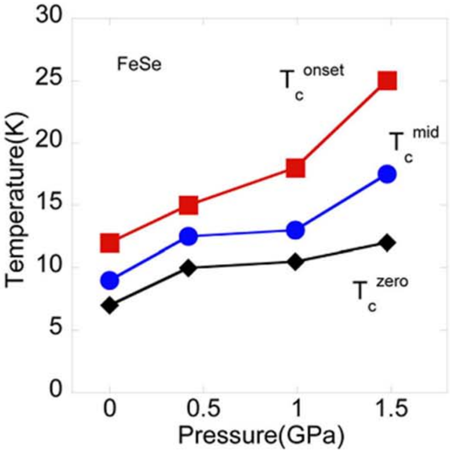


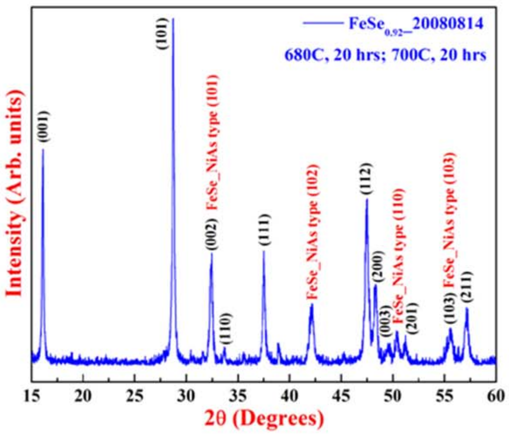
Tetragonal
P4/nmm

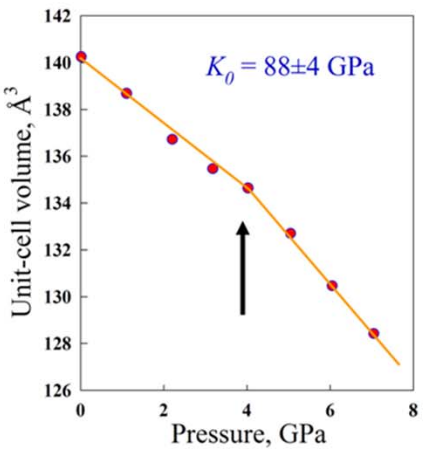


Tetragonal
P4/nmm









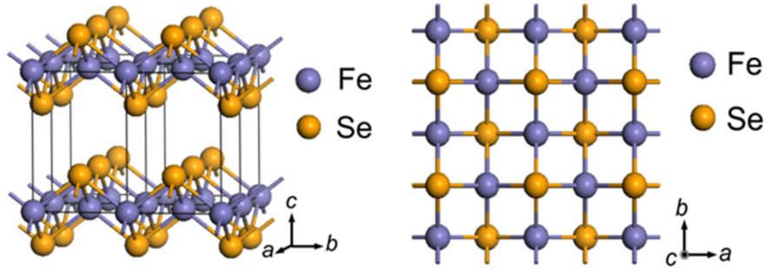
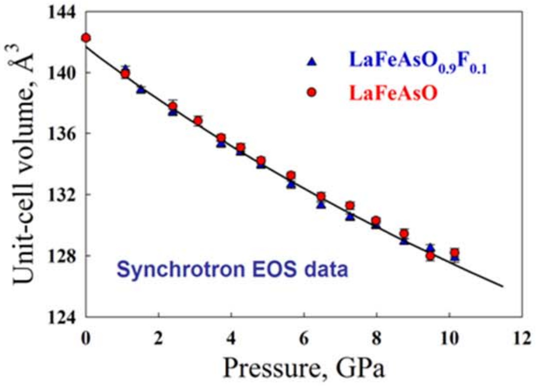
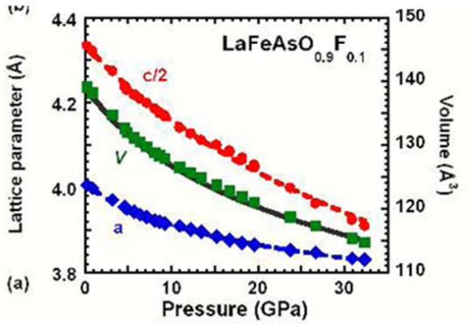
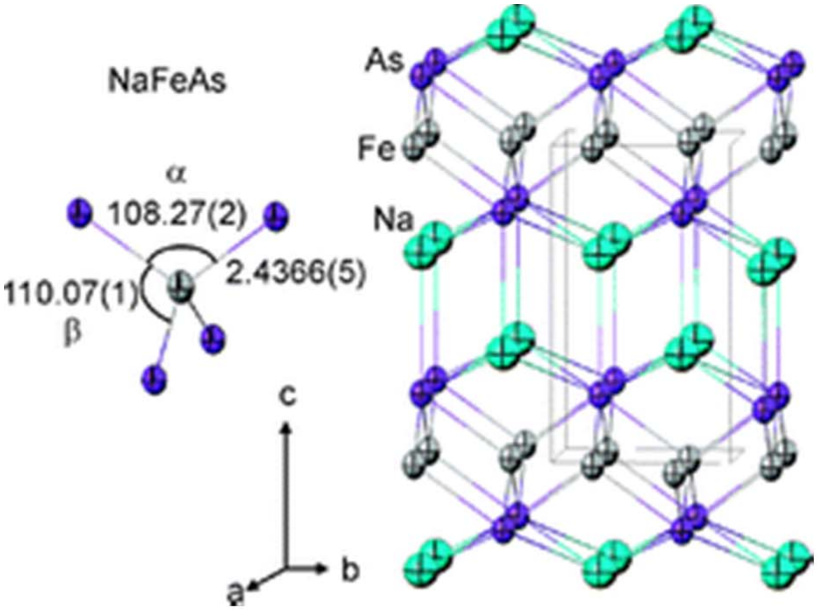


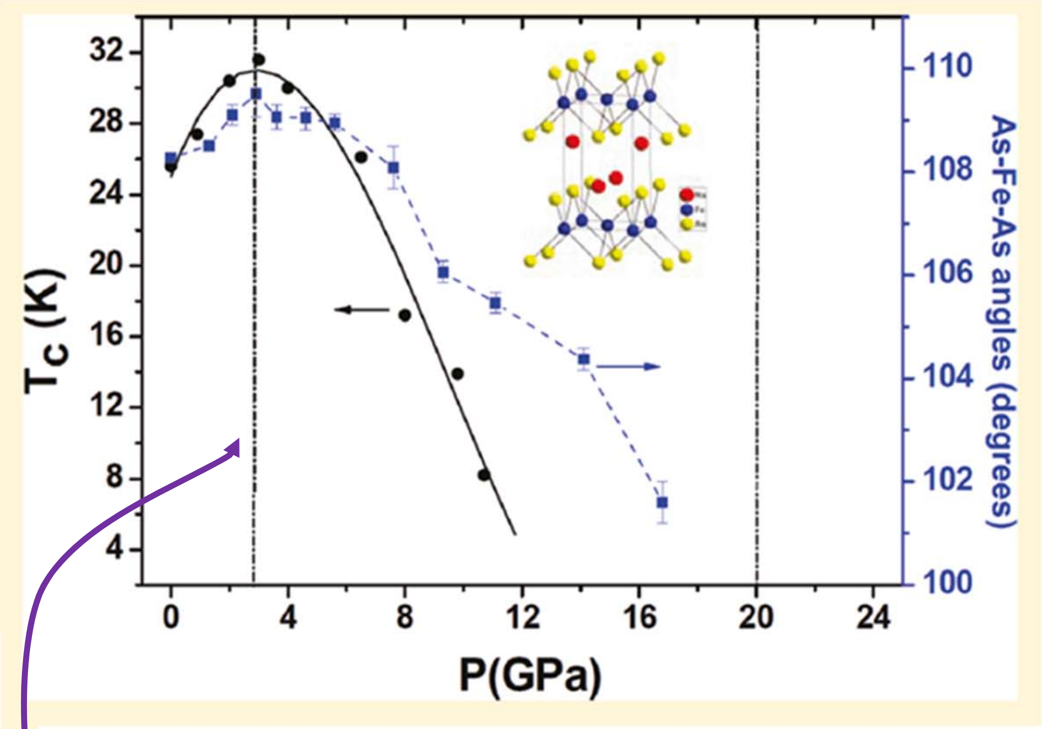
Figure 1 | Schematic crystal structure of α-FeSe. Four unit cells are shown to

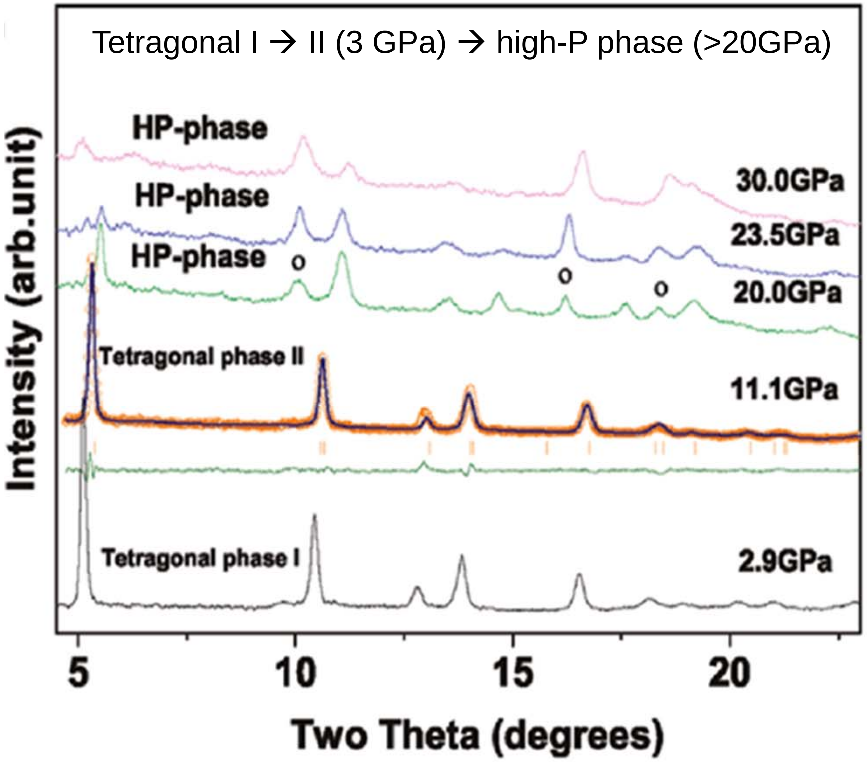


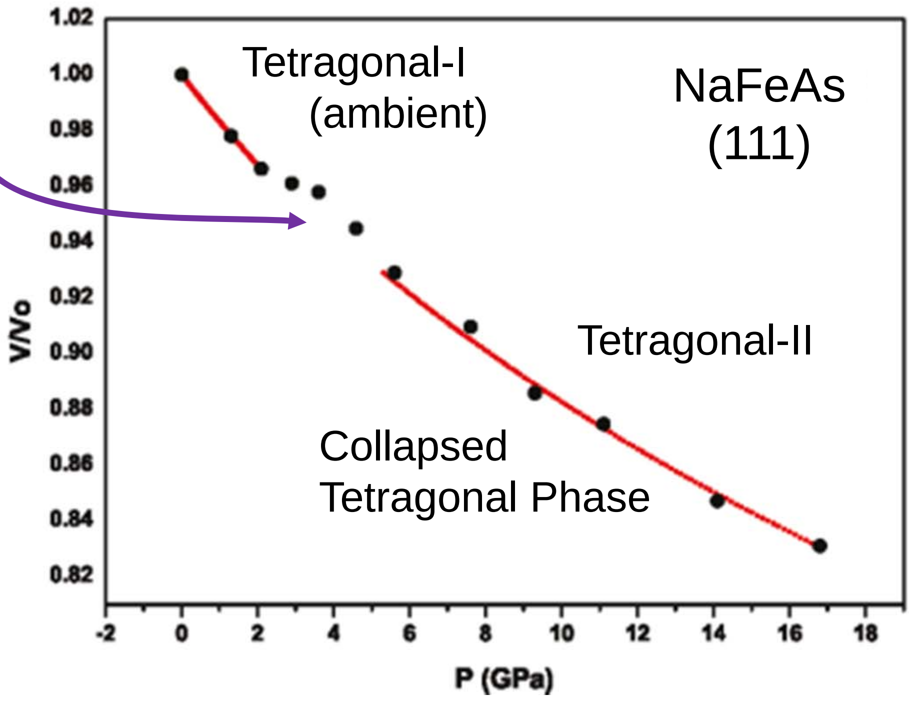
Neutron diffraction EOS data for $LaO_{0.9}F_{0.1}FeAs$
Note that there is a kink at about 4 GPa







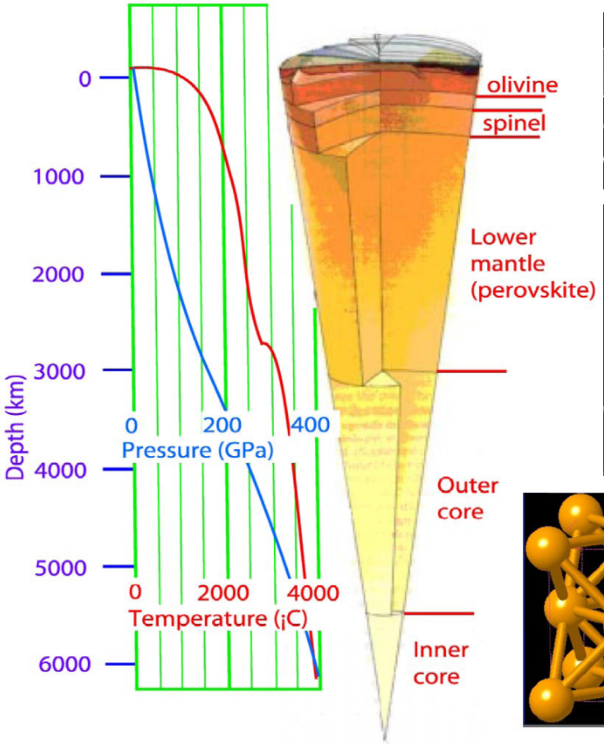

Tetragonal I → II (3 GPa) → high-P phase (>20GPa)

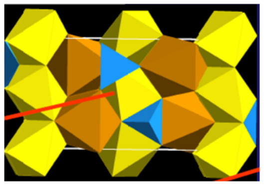

Tetragonal-I
(ambient)

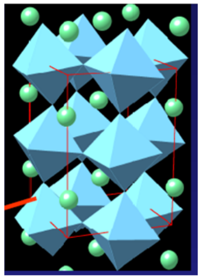
NaFeAs
(111)

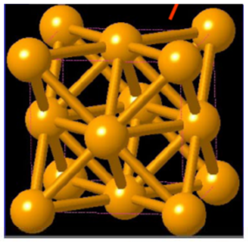
Tetragonal-II

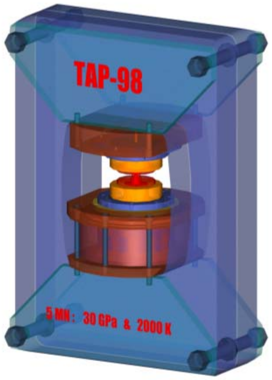
Collapsed
Tetragonal Phase

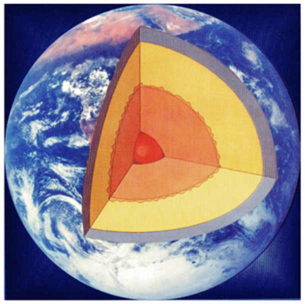


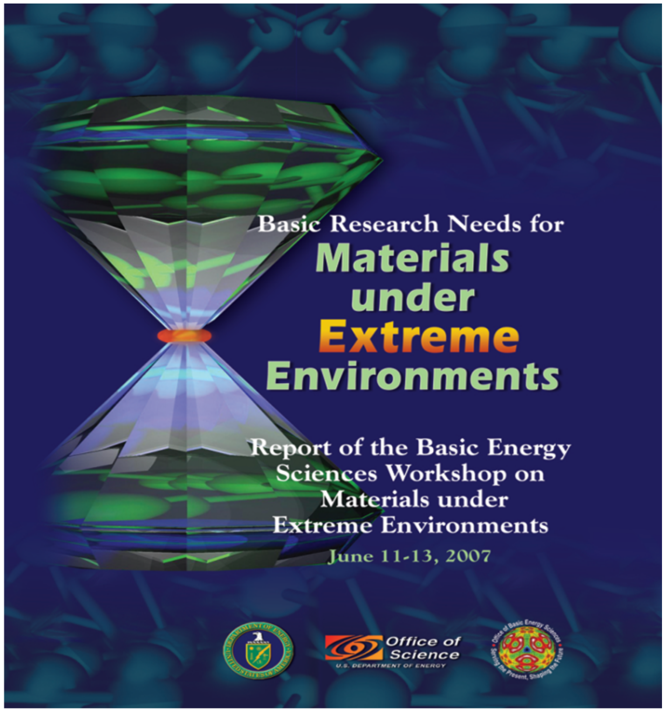








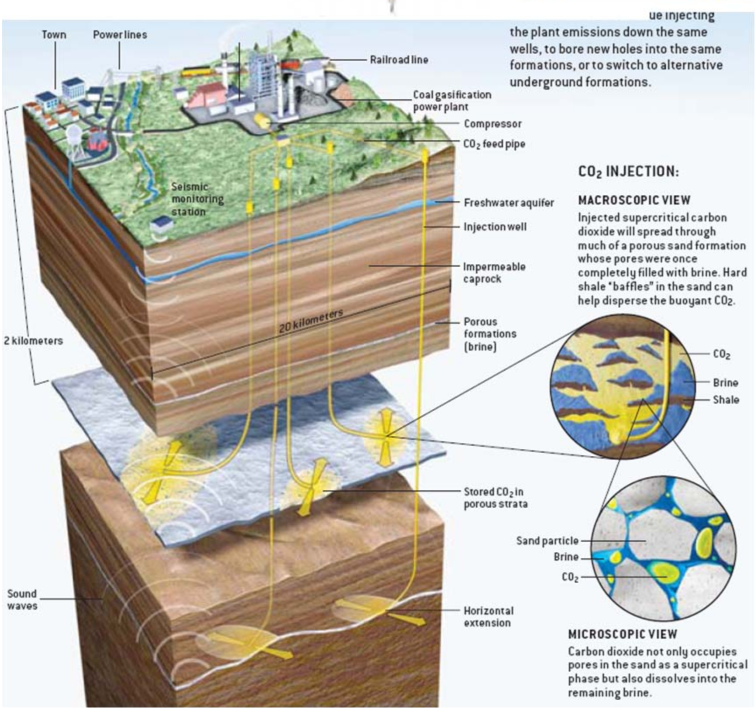



Basic Research Needs for

Materials under Extreme Environments

Report of the Basic Energy Sciences Workshop on Materials under Extreme Environments

June 11-13, 2007


ue injecting the plant emissions down the same wells, to bore new holes into the same formations, or to switch to alternative underground formations.

CO_2 INJECTION:

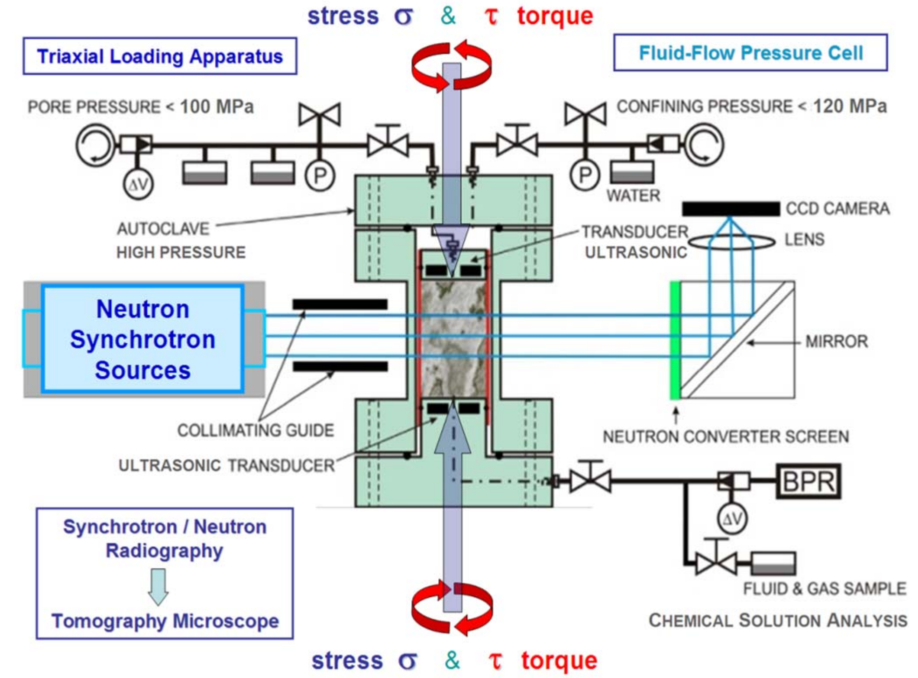
MACROSCOPIC VIEW

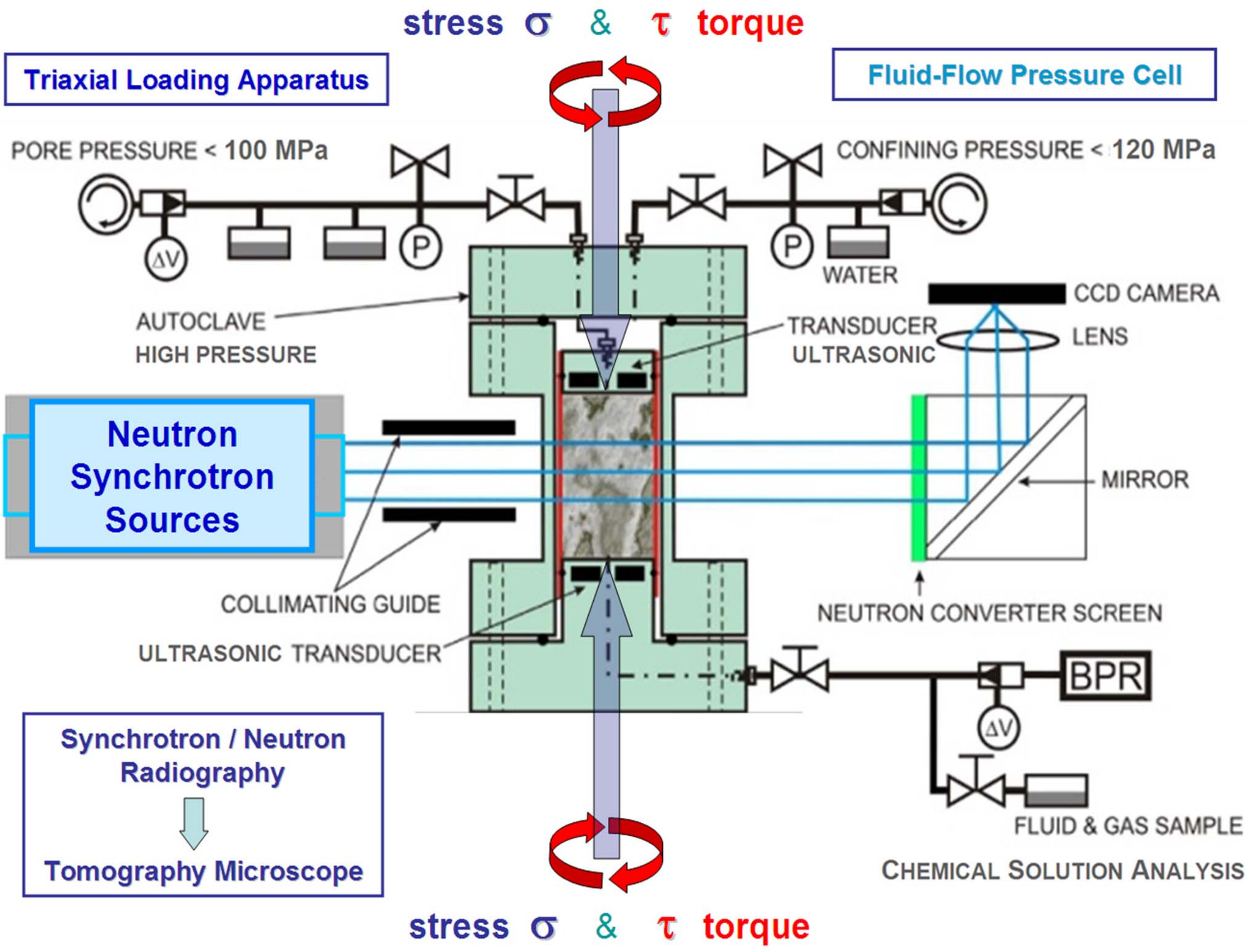
Injected supercritical carbon dioxide will spread through much of a porous sand formation whose pores were once completely filled with brine. Hard shale "baffles" in the sand can help disperse the buoyant CO_2.

MICROSCOPIC VIEW

Carbon dioxide not only occupies pores in the sand as a supercritical phase but also dissolves into the remaining brine.

Perturbations to The System
Away from its equilibriums





stress σ & τ torque

Triaxial Loading Apparatus

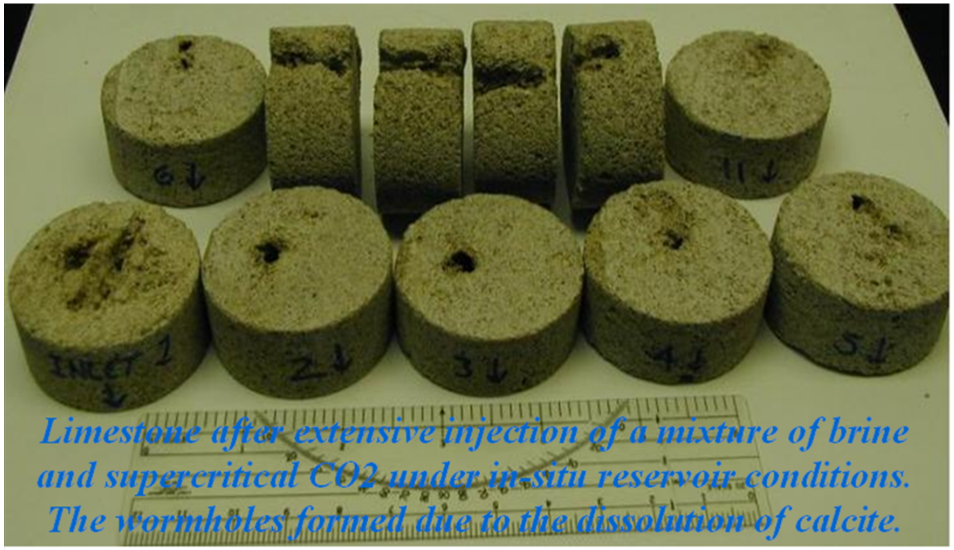
Fluid-Flow Pressure Cell

Synchrotron / Neutron Radiography

⇩

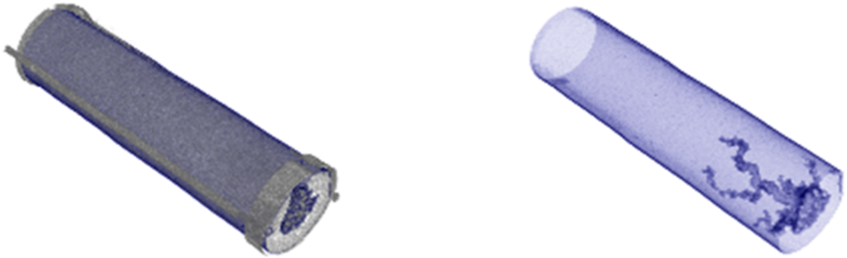
Tomography Microscope

stress σ & τ torque



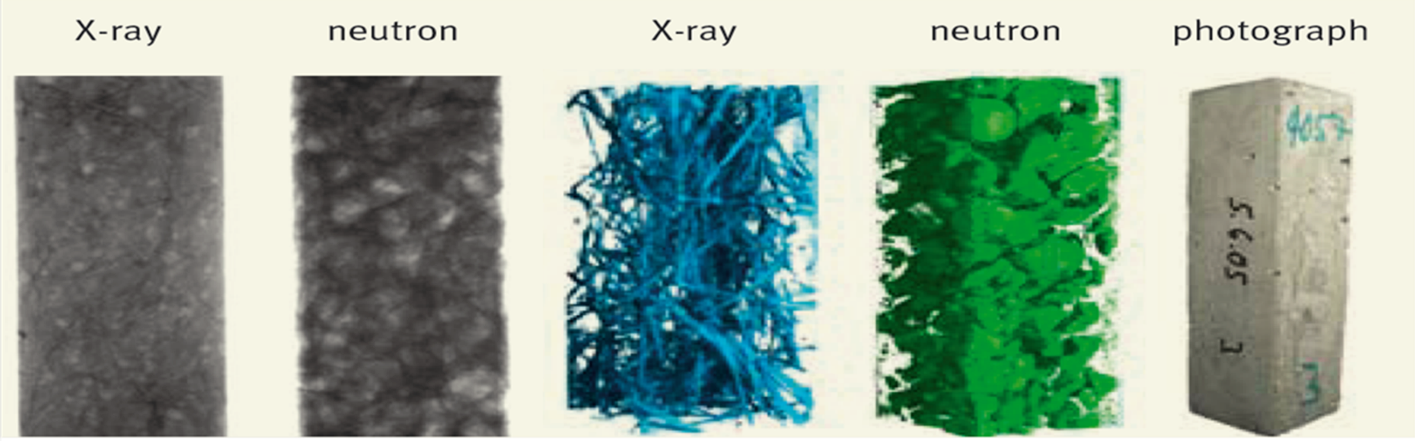
Limestone after extensive injection of a mixture of brine and supercritical CO2 under in-situ reservoir conditions. The wormholes formed due to the dissolution of calcite.

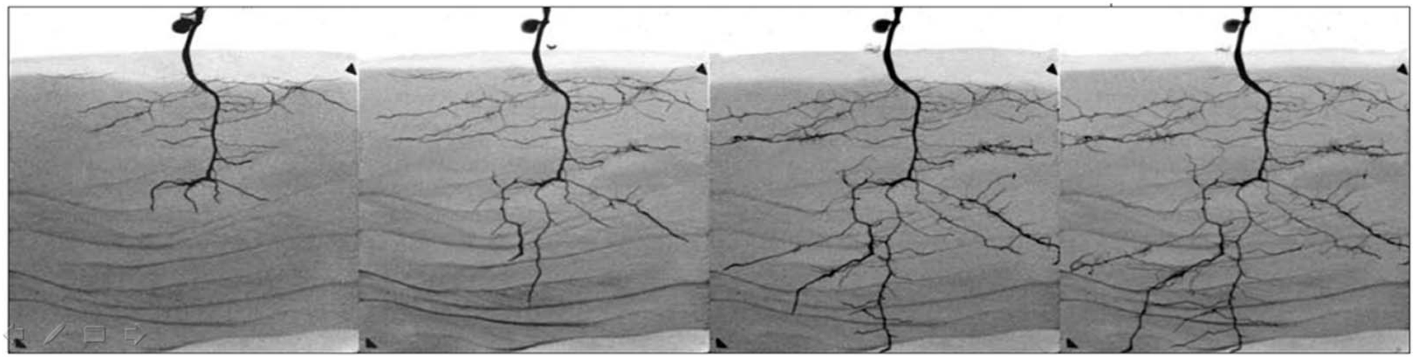
Neutron Tomography of Limestone After Stage 1 Flooding

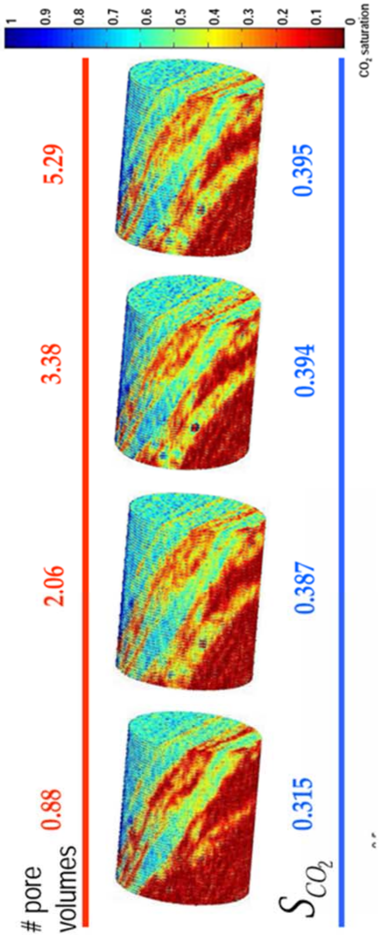


Outer Surface of Core

3-D Wormhole View

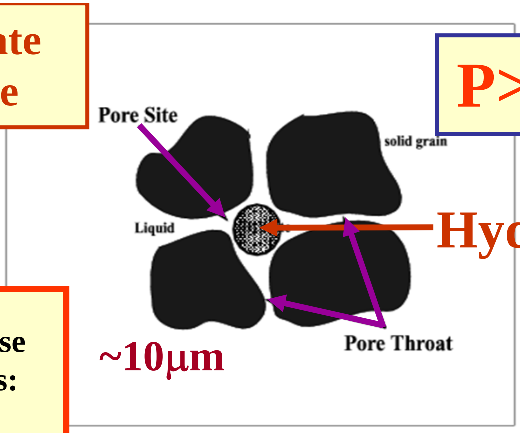






Pore-Network Schematics Traps for gas and water

Hydrate stable



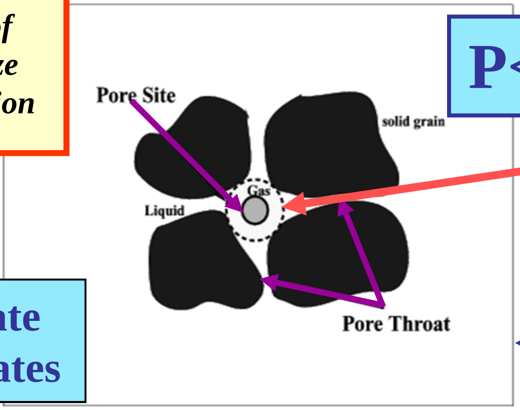
$P>P_d$

Hydrate

~10µm

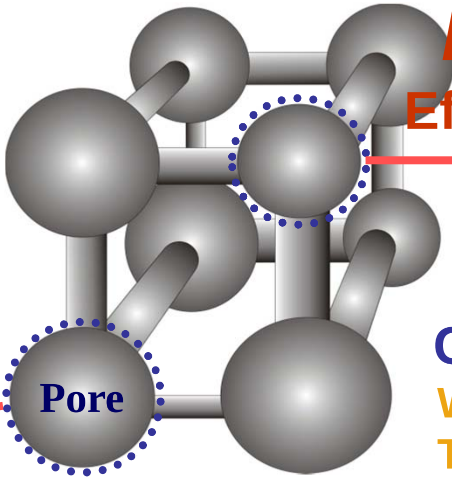
Gas Phase Patterns:

Effect of Pore-Size Distribution

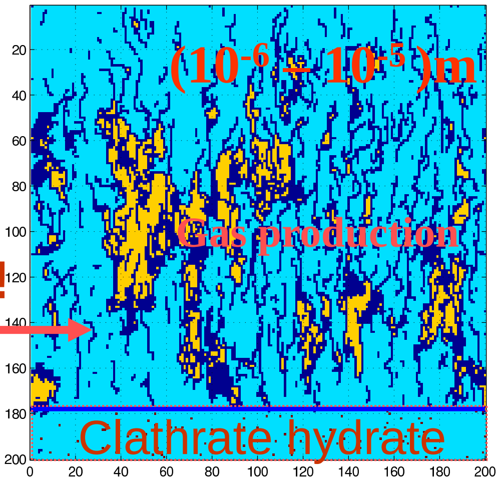


$P<P_d$

Hydrate dissociates



***P-T* Effects!**



$(10^{-6} - 10^{-5})$m

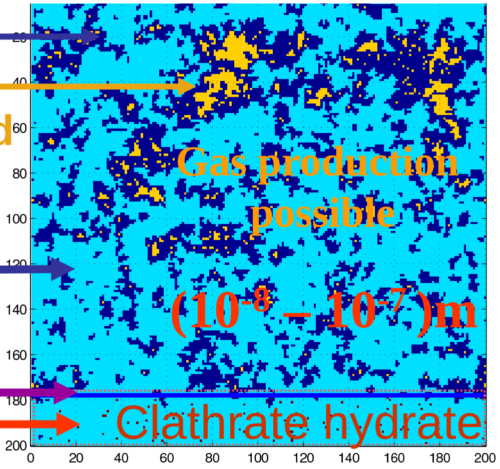
Gas production

Clathrate hydrate

CH4

Water

Trapped



Gas production possible

$(10^{-8} - 10^{-7})$m

Clathrate hydrate

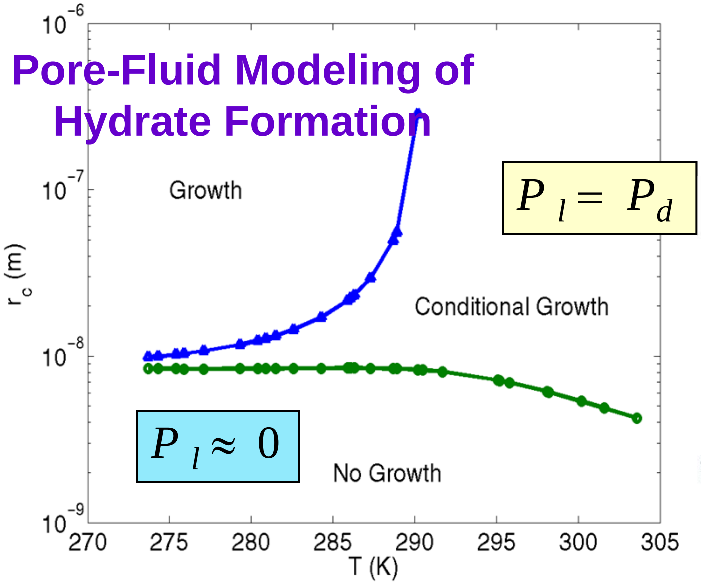
$P<P_d$

$P=P_d$

$P>P_d$

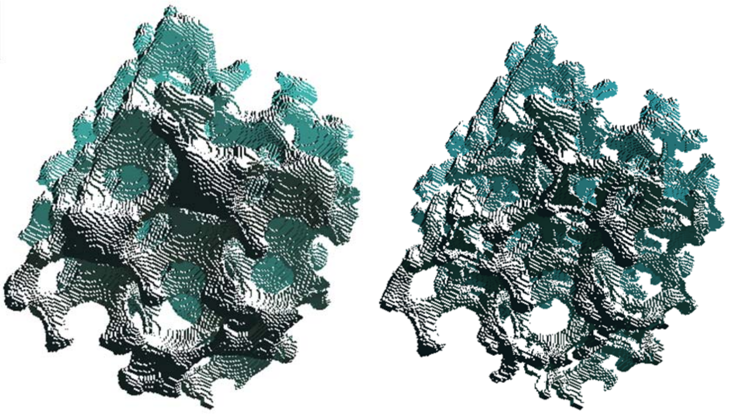
Hydrate Dissociation in a Single Pore

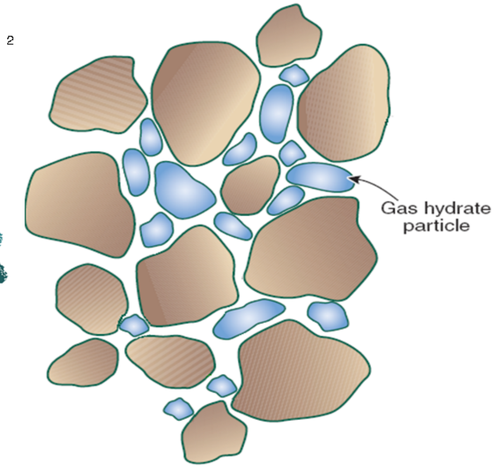
Pore-Fluid Modeling of Hydrate Formation



$P_l = P_d$

$P_l \approx 0$





Curiosity versus **Mission**
(interest and responsibility)

Real Field Tests

Large Scale Model

Geo-hydrology

纳米力学性质

diffraction

相邻分布函数

Implementation

Simulation

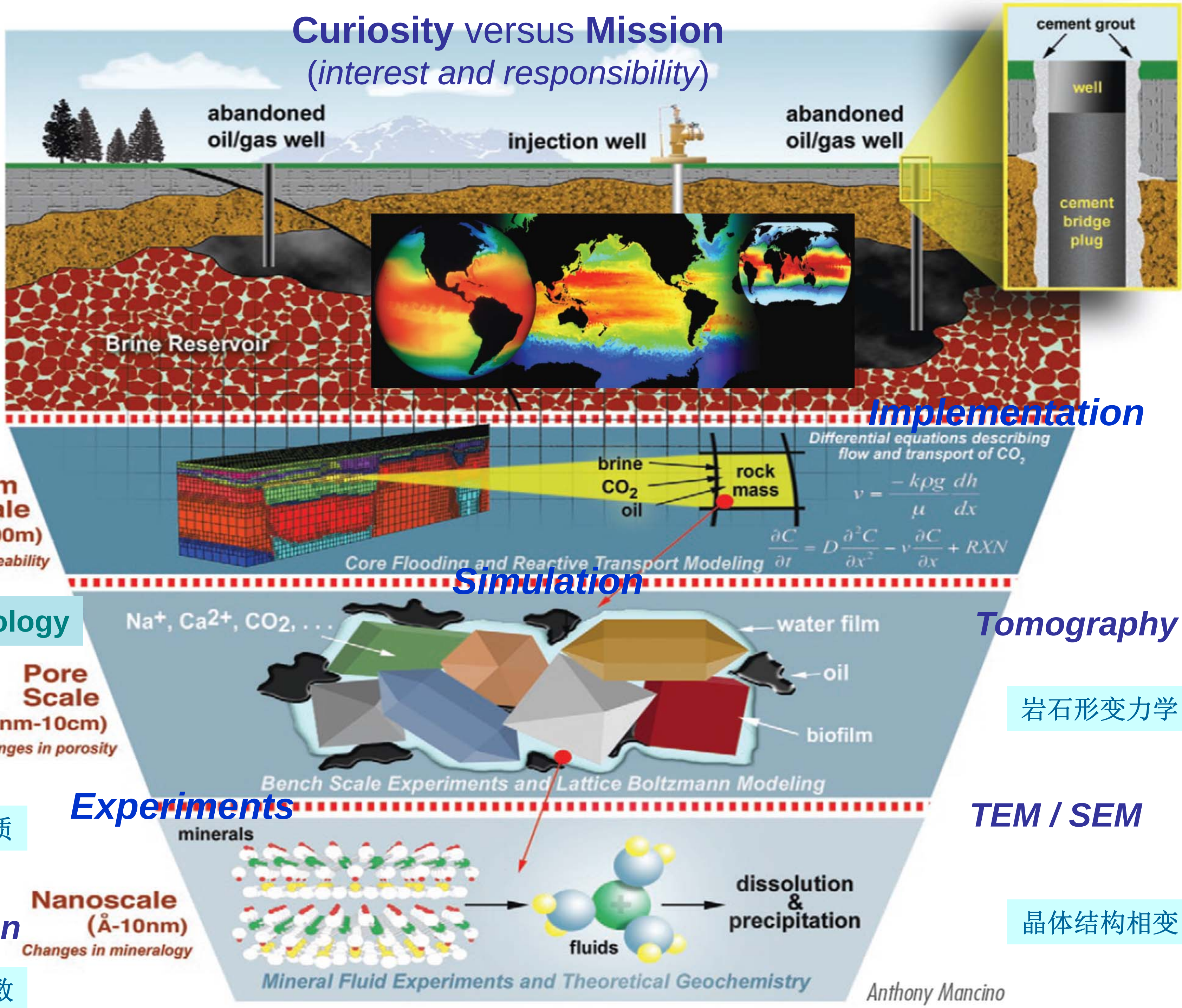
Experiments

Tomography

岩石形变力学

TEM / SEM

晶体结构相变

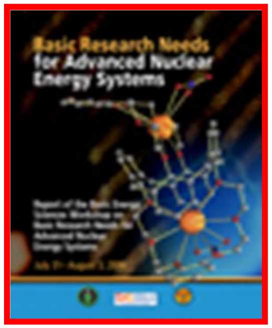


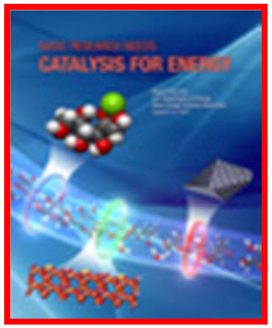
Basic Research Needs to Assure a Secure Energy Future

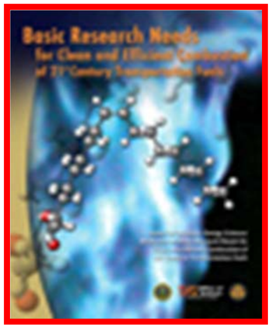
• Energy Independence • Environmental Sustainability • Economic Opportunity •


BASIC RESEARCH NEEDS
TO ASSURE
A SECURE ENERGY FUTURE

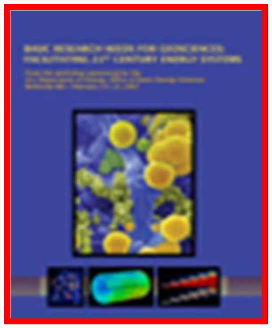
A Report from the
Basic Energy Sciences Advisory Committee

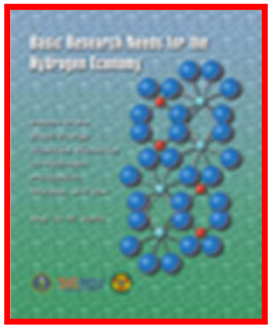

Basic Research Needs for Advanced Nuclear Energy Systems


BASIC RESEARCH NEEDS
CATALYSIS FOR ENERGY

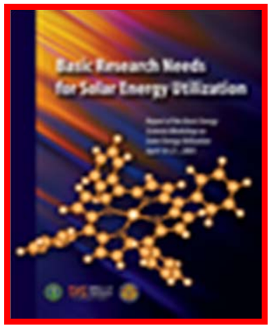

Basic Research Needs for Clean and Efficient Combustion of 21st Century Transportation Fuels


Basic Research Needs for Electrical Energy Storage


BASIC RESEARCH NEEDS FOR GEOSCIENCES: FACILITATING 21ST CENTURY ENERGY SYSTEMS

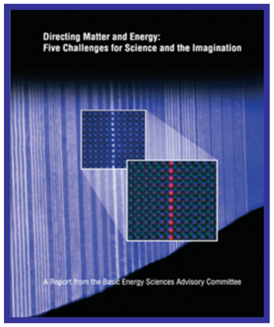

Basic Research Needs for the Hydrogen Economy


Basic Research Needs for Materials under Extreme Environments


Basic Research Needs for Solar Energy Utilization


BASIC RESEARCH NEEDS FOR SOLID-STATE LIGHTING


BASIC RESEARCH NEEDS FOR SUPERCONDUCTIVITY

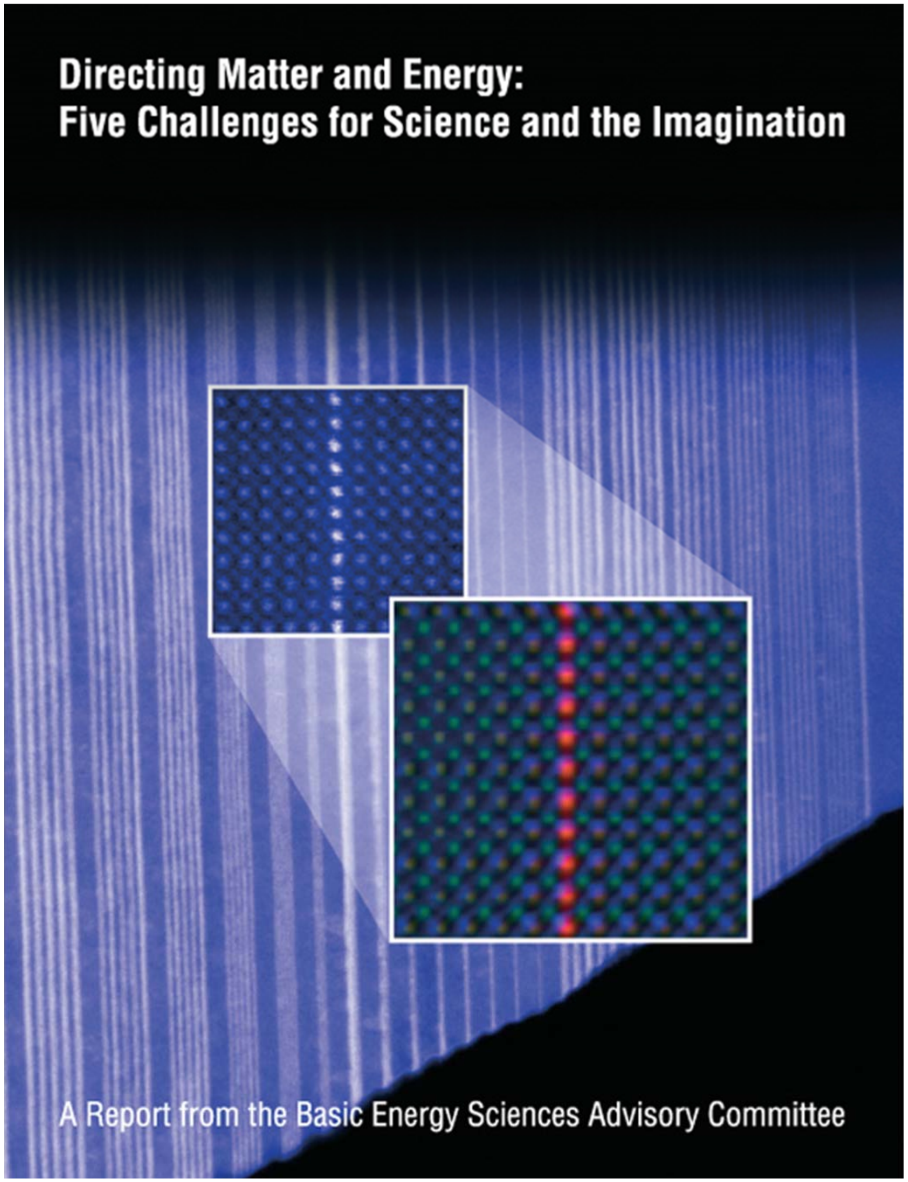

Directing Matter and Energy:
Five Challenges for Science and the Imagination

A Report from the Basic Energy Sciences Advisory Committee

DOE : Basic Research Needs

Advanced Nuclear Energy Systems; Catalysis for Energy; Combustion of 21st Century Fuels; Electric Energy Storage; Geosciences: Facilitating Energy Systems; Hydrogen Economy; Materials under Extreme Environments; Solar Energy Utilization; Solid-State Lighting; Superconductivity

Directing Matter and Energy: *Five Challenges for Science and the Imagination*

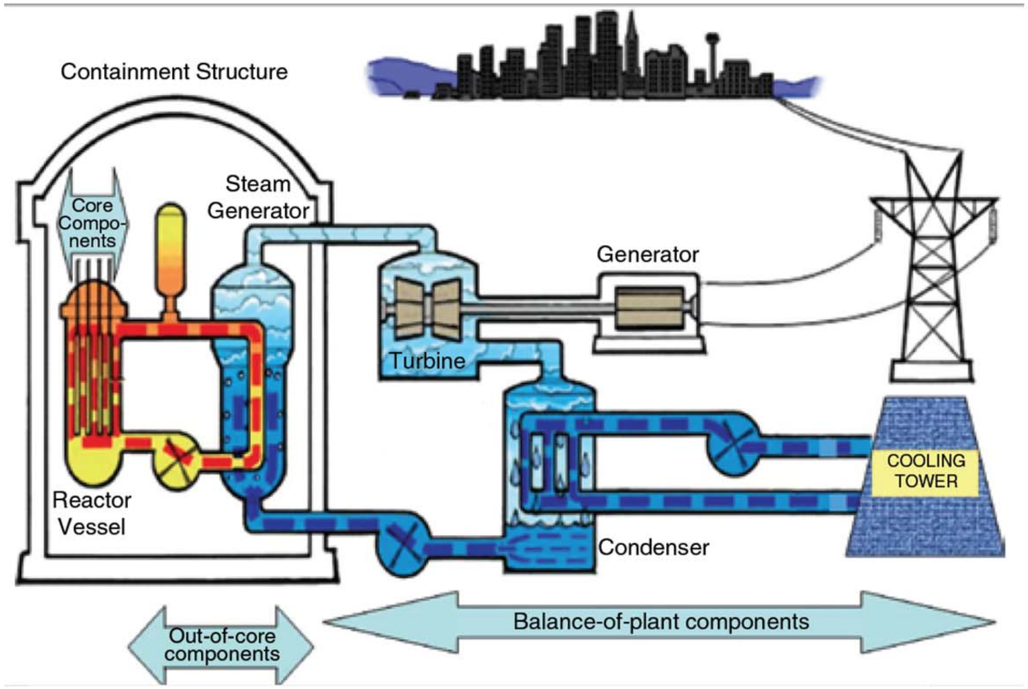


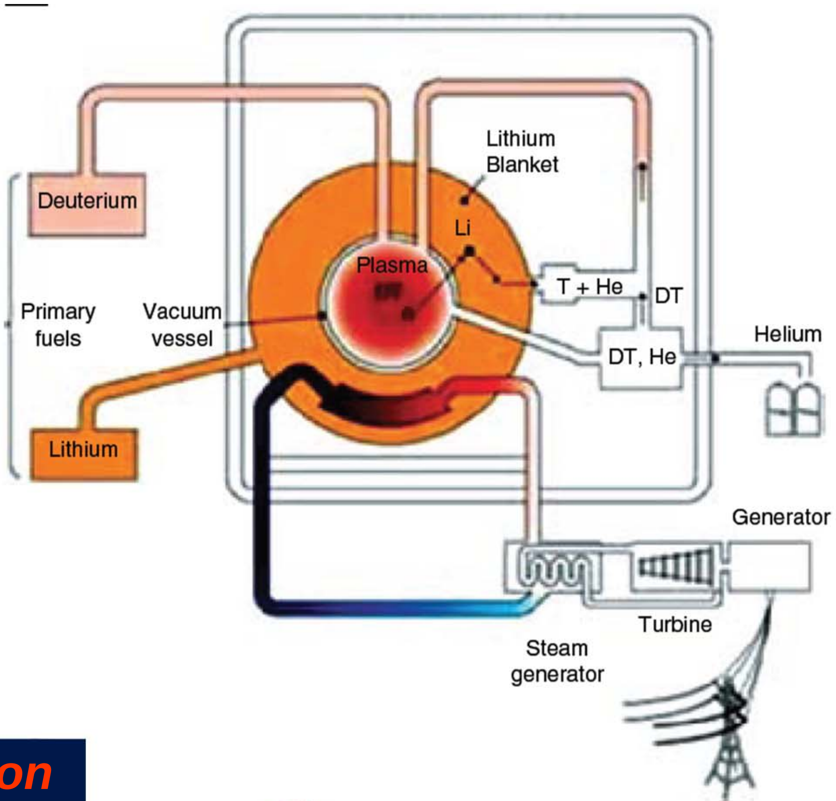
Directing Matter and Energy:
Five Challenges for Science and the Imagination

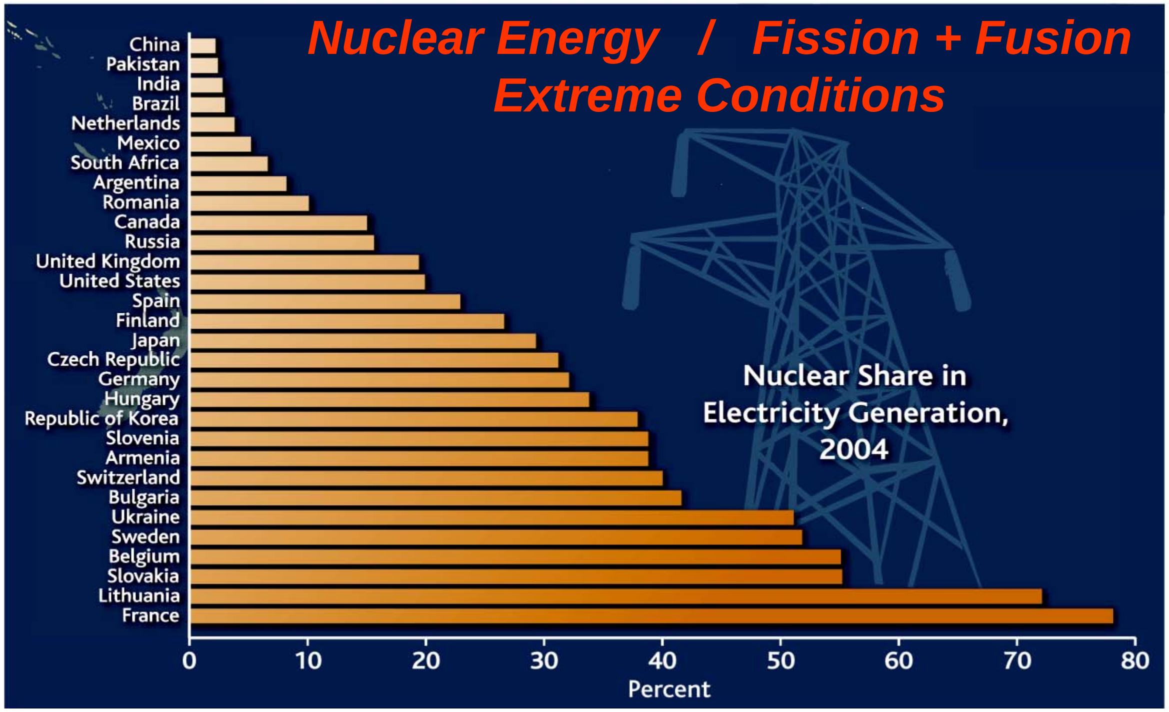
A Report from the Basic Energy Sciences Advisory Committee

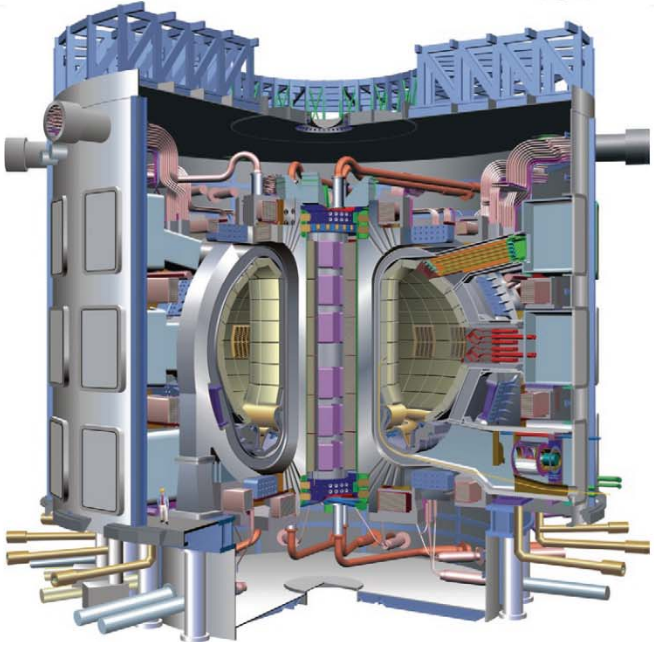
- ***How do we control material processes at the level of electrons?***
- ***How do we design and perfect atom- and energy- efficient synthesis of revolutionary new forms of matter with tailored properties?***
- ***How do remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents and how can we control these properties?***
- ***How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling the living things?***
- ***How do we characterize and control matter away — especially very far away — from equilibrium?***

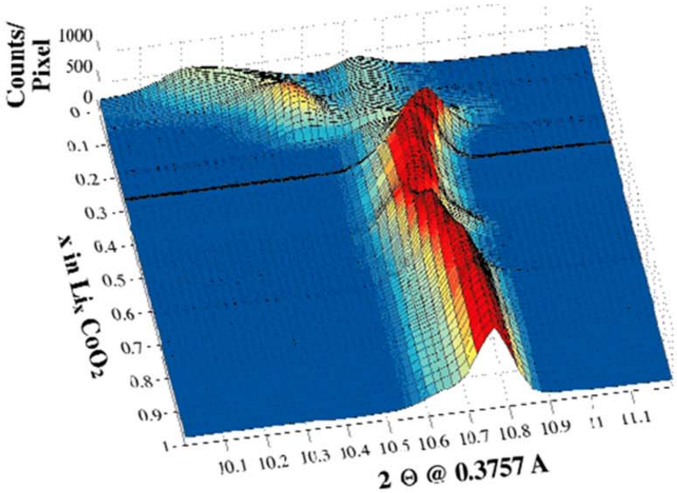
Nuclear Energy / Fission + Fusion
Extreme Conditions

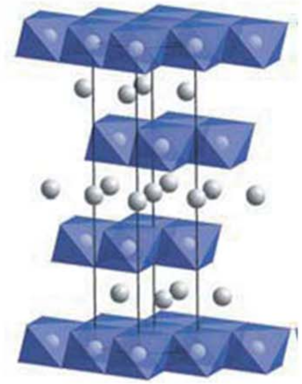


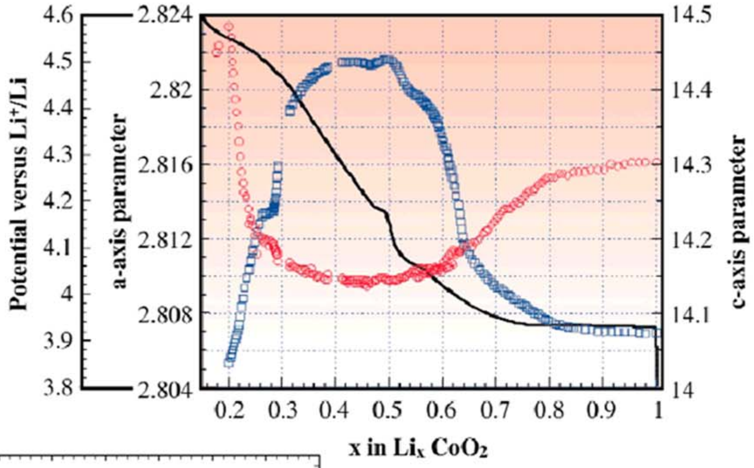




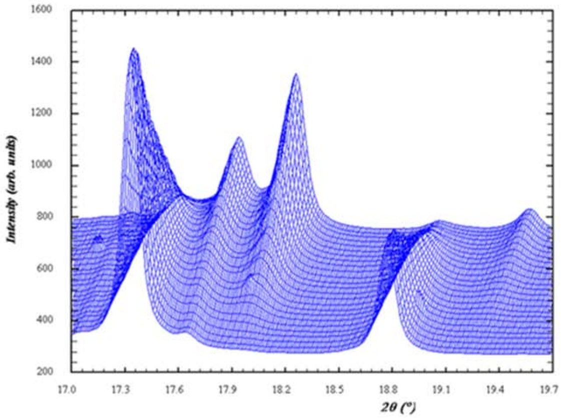




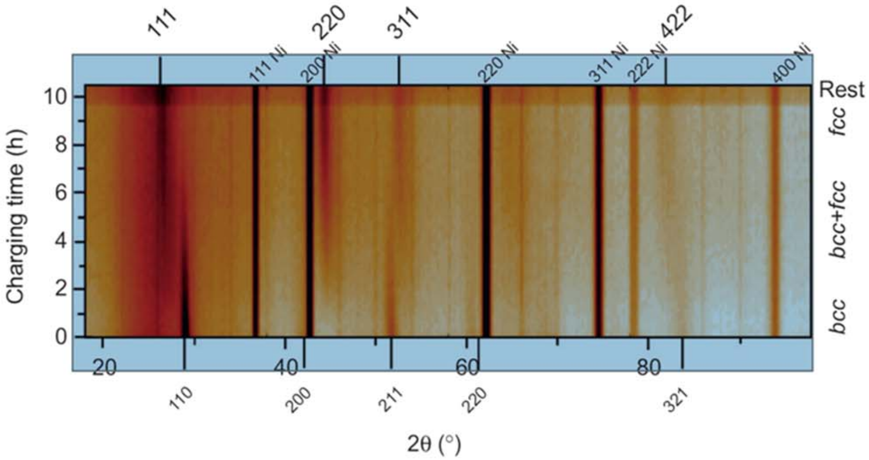


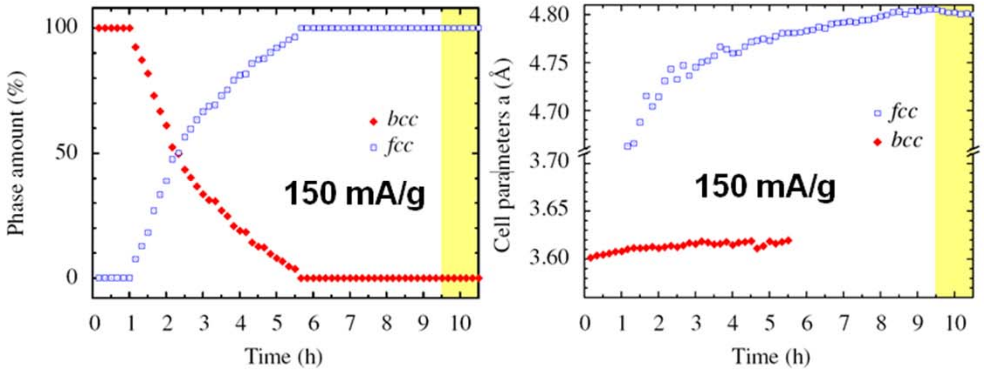


Diffraction study of battery electro-chemistry process and structural phase transformation in electrodes as a function of charge/discharge cycling to understand capacity mechanisms and to enhance battery performances.



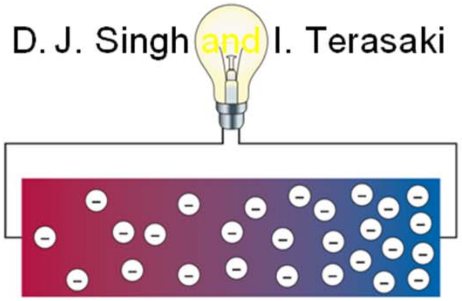
Evolution of the diffraction pattern from a LiFePO4 electrode during fast discharge

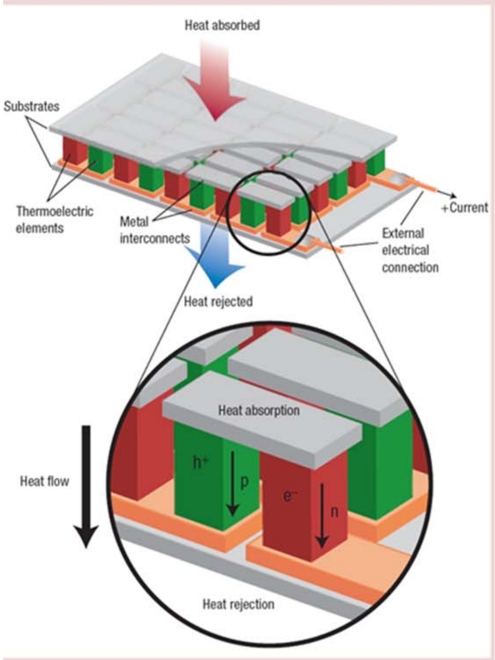




2D projection of the neutron diffraction pattern intensities as function of time during electrochemical charge of Pd-doped Mg0.65Sc0.35 active material showing the progressive transformation from *bcc* to *fcc*. Evolution of the phase amount and unit cell for the *bcc* and the *fcc* phases during charge.

D. J. Singh and I. Terasaki





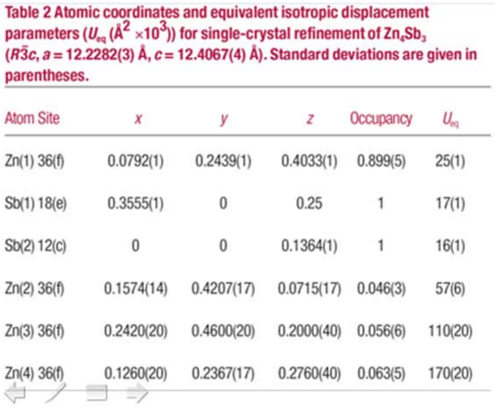
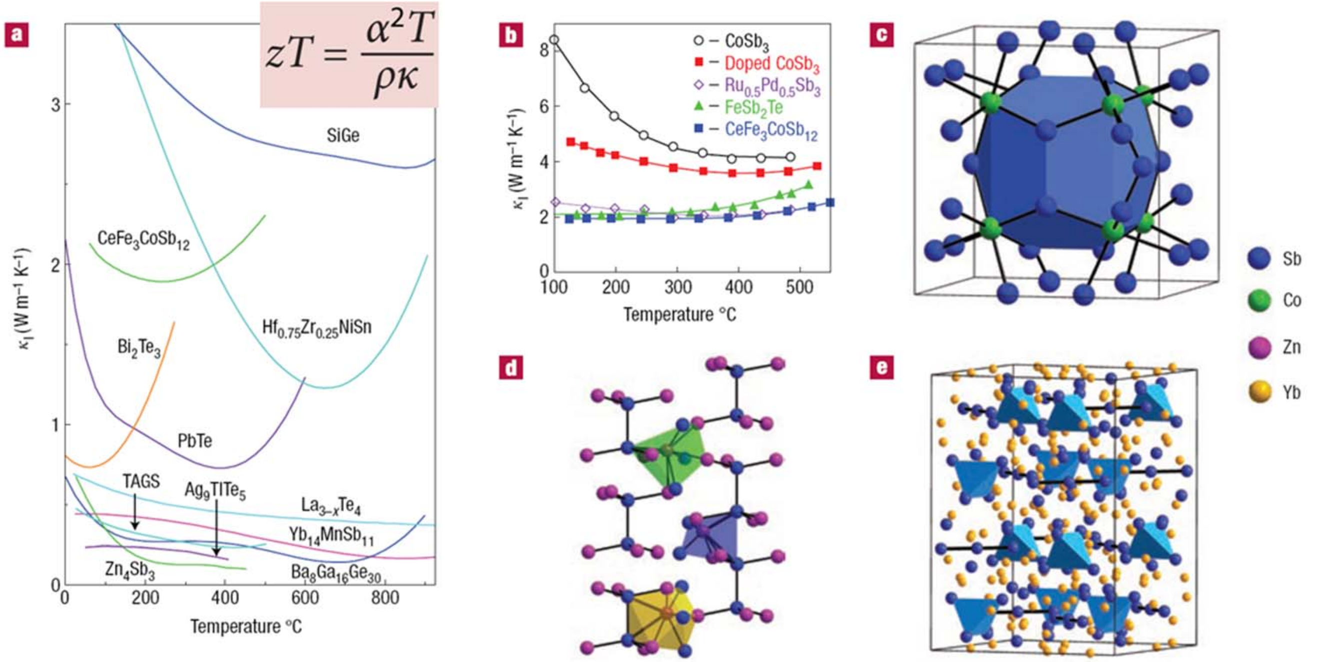


Table 2 Atomic coordinates and equivalent isotropic displacement parameters (U_{eq} (Å^2 ×10^3)) for single-crystal refinement of Zn_4Sb_3 ($R\bar{3}c$, $a = 12.2282(3)$ Å, $c = 12.4067(4)$ Å). Standard deviations are given in parentheses.

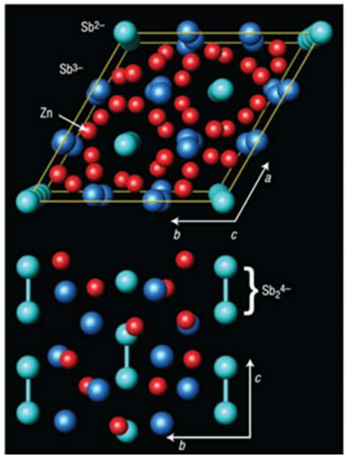
Atom Site	*x*	*y*	*z*	Occupancy	U_{eq}
Zn(1) 36(f)	0.0792(1)	0.2439(1)	0.4033(1)	0.899(5)	25(1)
Sb(1) 18(e)	0.3555(1)	0	0.25	1	17(1)
Sb(2) 12(c)	0	0	0.1364(1)	1	16(1)
Zn(2) 36(f)	0.1574(14)	0.4207(17)	0.0715(17)	0.046(3)	57(6)
Zn(3) 36(f)	0.2420(20)	0.4600(20)	0.2000(40)	0.056(6)	110(20)
Zn(4) 36(f)	0.1260(20)	0.2367(17)	0.2760(40)	0.063(5)	170(20)

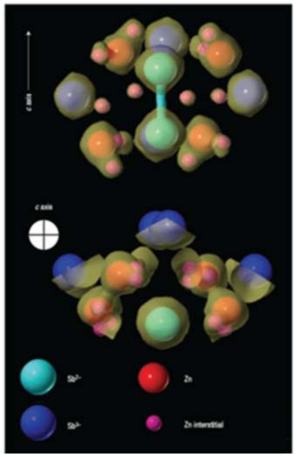
G. Jeffrey Snyder* et al. (2004, 2008) --- Caltech ---

Thermoelectric materials can generate electricity from waste heat or be used as solid-state Peltier coolers. Identifying materials with high thermoelectric efficiency by tuning alloys' composition and structure, thus controlling simultaneously the electric and thermal properties.

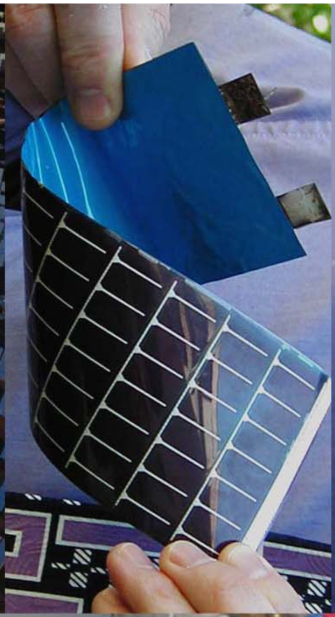


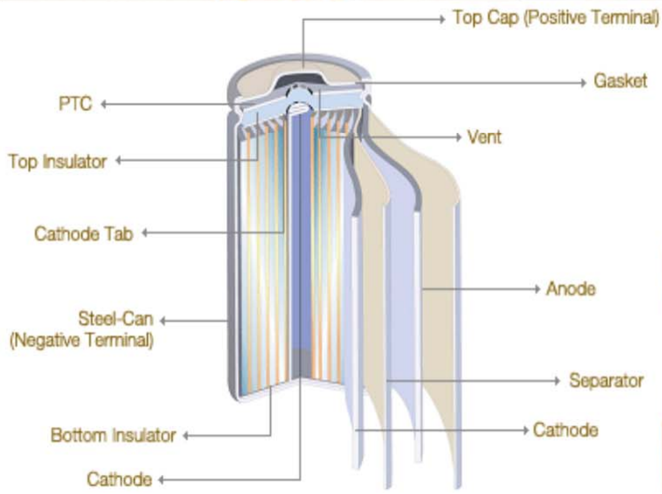
$$zT = \frac{\alpha^2 T}{\rho \kappa}$$

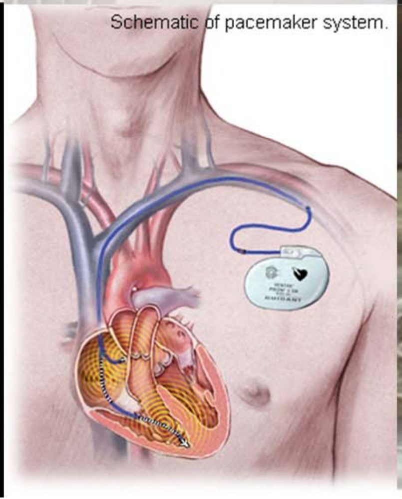


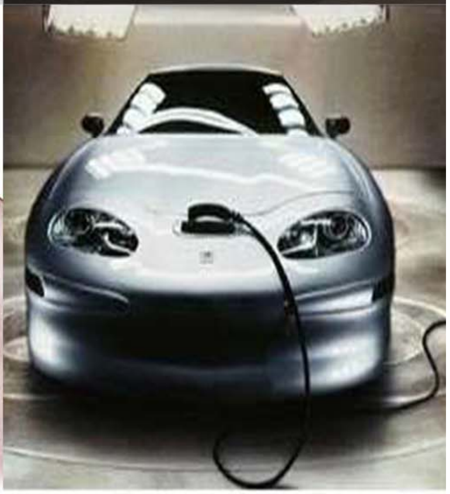


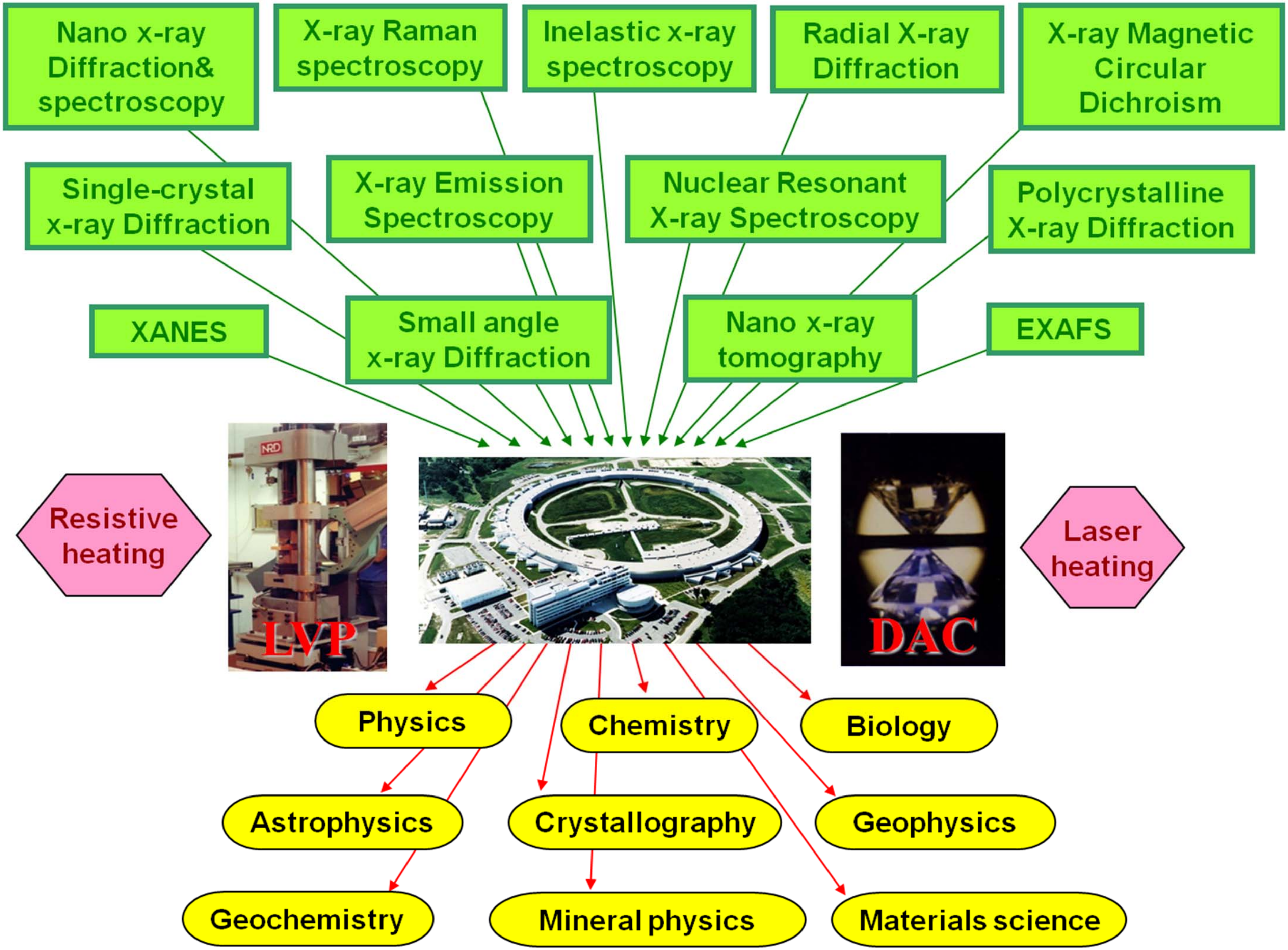
Diffraction studies reveals unique structural features that control both electronic and thermal properties of Zn4Sb3. Valence semiconductor, structure disorder, and glass-like interstitial sites are highly effective for an ideal 'phonon glass, electron crystal' thermoelectric material.






Schematic of pacemaker system.





Nano x-ray Diffraction& spectroscopy

X-ray Raman spectroscopy

Inelastic x-ray spectroscopy

Radial X-ray Diffraction

X-ray Magnetic Circular Dichroism

Single-crystal x-ray Diffraction

X-ray Emission Spectroscopy

Nuclear Resonant X-ray Spectroscopy

Polycrystalline X-ray Diffraction

XANES

Small angle x-ray Diffraction

Nano x-ray tomography

EXAFS

Resistive heating

LVP

DAC

Laser heating

Physics

Chemistry

Biology

Astrophysics

Crystallography

Geophysics

Geochemistry

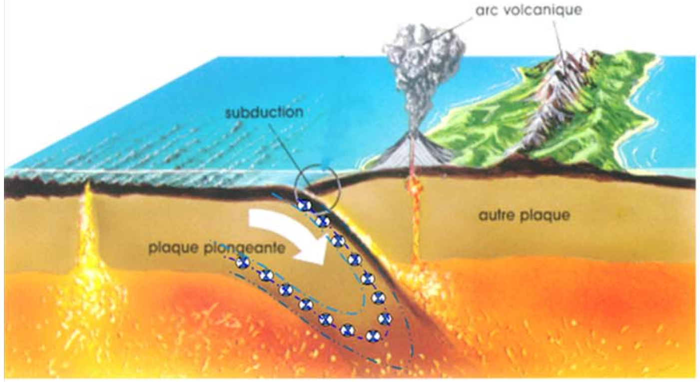
Mineral physics

Materials science

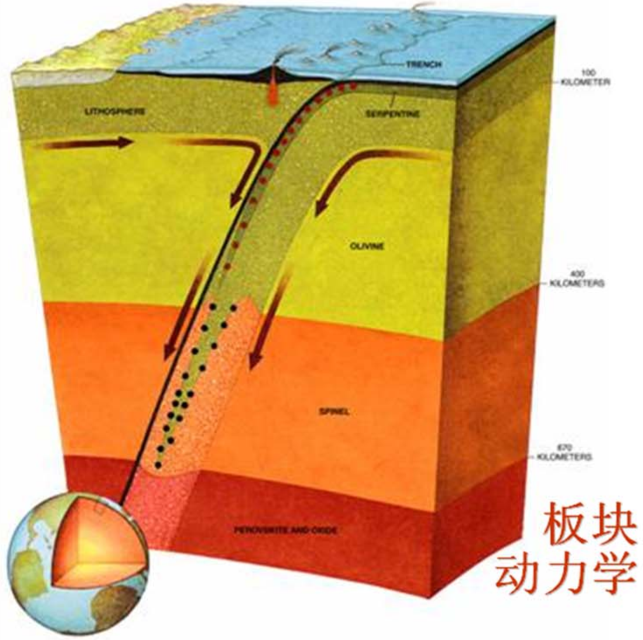
高温高压中子衍射实验研究深部地球含水矿物

晶体化学, 热力学稳定性, 地震断层力学

火山学 :*矿物脱水所致部分融熔 !*

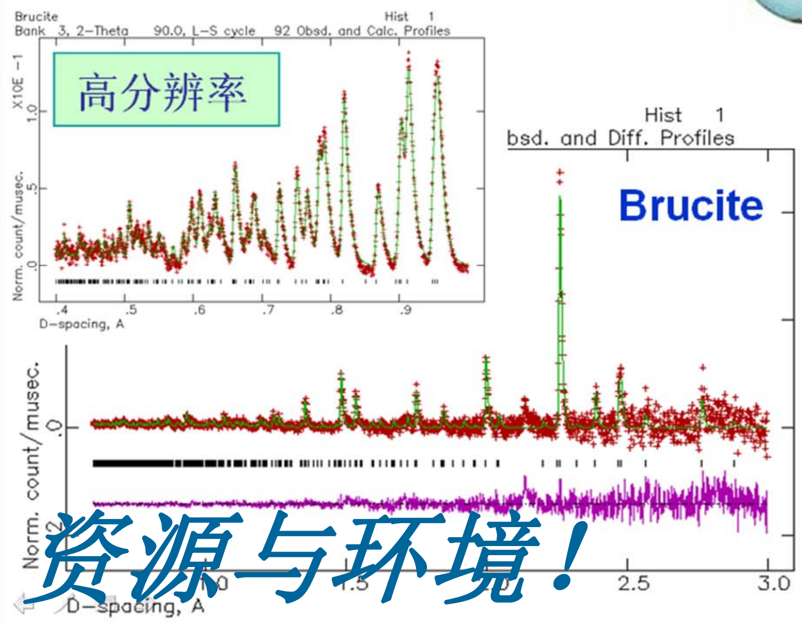


地震学 : *矿物脱水所致*
脆性断裂 ?!



板块
动力学

高压下的铁镍相

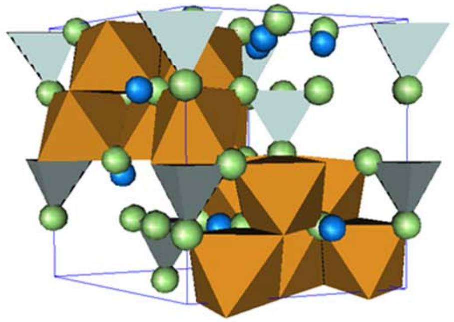


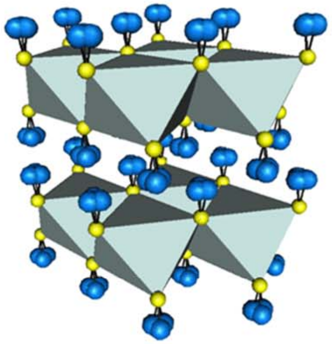
高分辨率

资源与环境 !

高温高压下合成含水矿物

Phase_A : $Mg_7Si_2O_8(OD)_6$



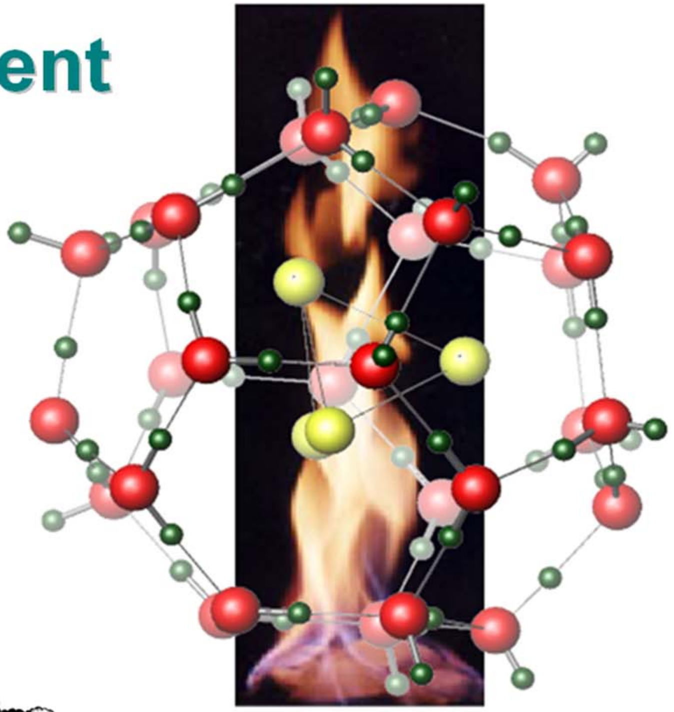


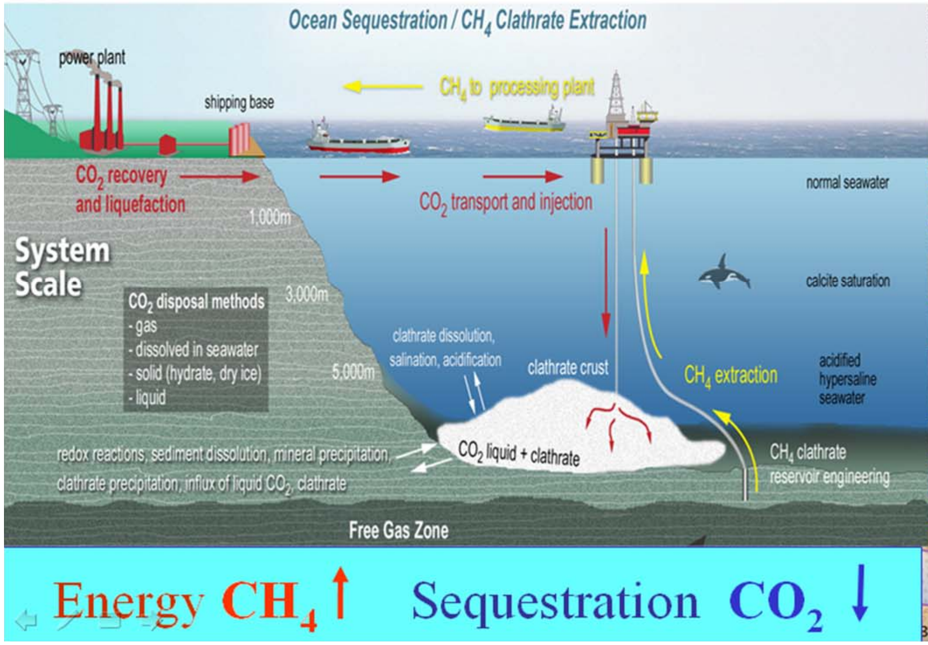
Brucite : $Mg(OH)_2$

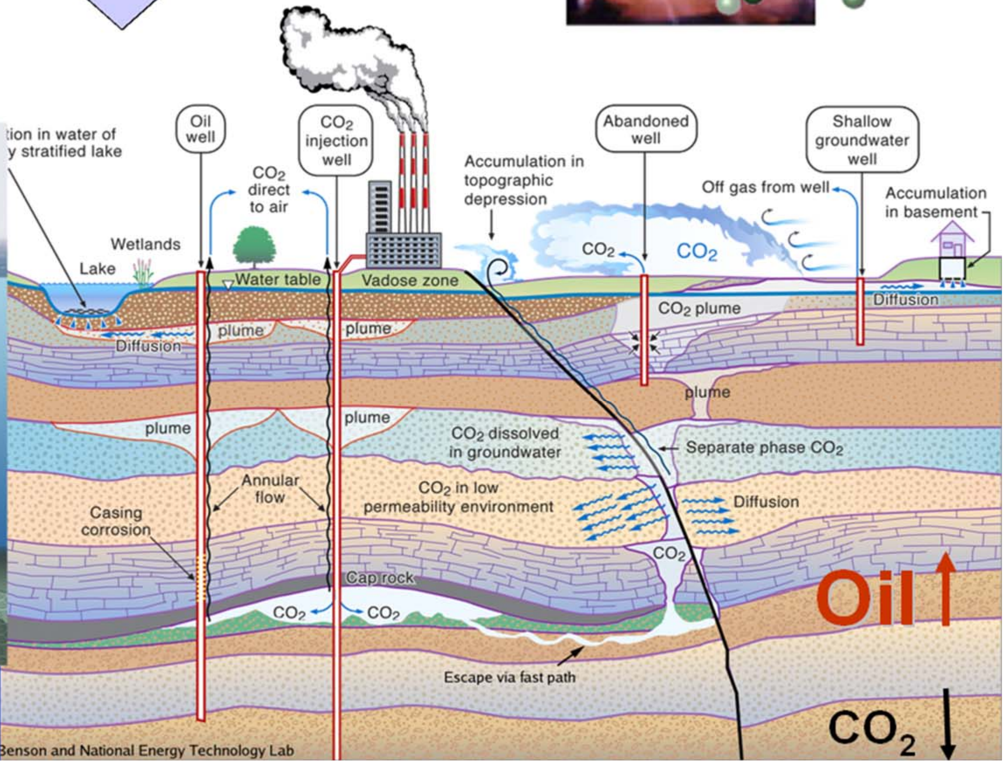
高温高压下含水矿物
的中子衍射实验研究

全球水循环 和 全球碳循环 的 科学研究 ?!

Clean Energy & Clean Environment







Coal → $H_2 + CO_2$

Gas saturated water stream

high-P feed in flue gas

hydrate "reaction"
@ P=300bar & T=3°C

Chiller Reactor

Purifier (remove SO_2 & H_2S)

Gas Separation, Purification,
Storage, and Transportation

Separation of H_2 gas and
CO_2 clathrate slurry
>67% CO_2 captured in hydrate

Flash Reactor

selective capture CO_2
and separate H_2/water

DOE goal of >92% CO_2 capture

Call for R&D on "Promoters"

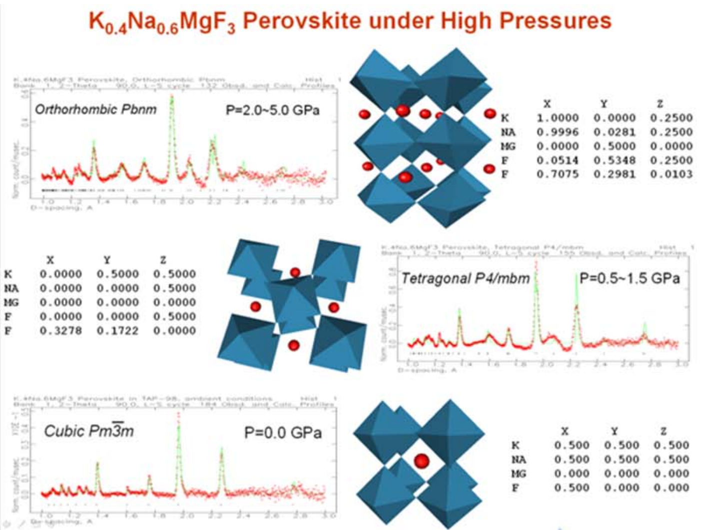
FUTUREGEN
A Prototype of Tomorrow's
Coal-Fueled Power Plant

LANL project
funded by
DOE-FE

Storages

H_2 Transportation
CO_2 sequestration

Effective route to separate H_2 & CO_2


$K_{0.4}Na_{0.6}MgF_3$ Perovskite under High Pressures

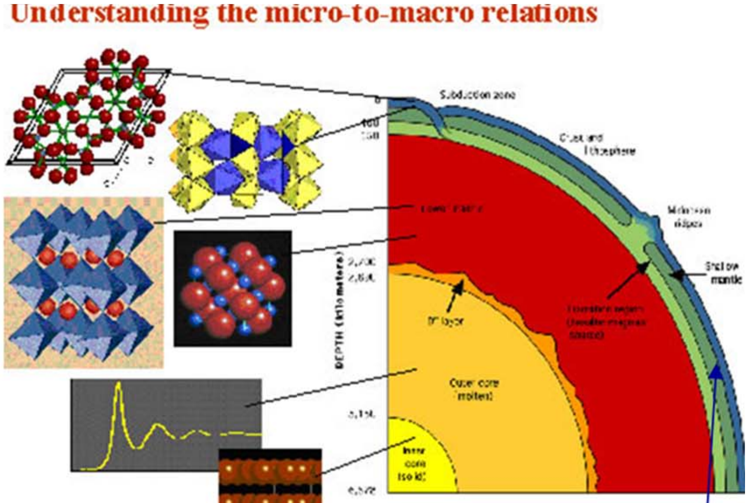
	X	Y	Z
K	1.0000	0.0000	0.2500
NA	0.9996	0.0281	0.2500
MG	0.0000	0.5000	0.0000
F	0.0514	0.5348	0.2500
F	0.7075	0.2981	0.0103

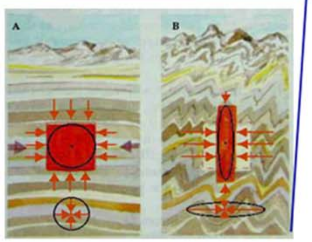
	X	Y	Z
K	0.0000	0.5000	0.5000
NA	0.0000	0.5000	0.5000
MG	0.0000	0.0000	0.0000
F	0.0000	0.0000	0.5000
F	0.3278	0.1722	0.0000

	X	Y	Z
K	0.500	0.500	0.500
NA	0.500	0.500	0.500
MG	0.000	0.000	0.000
F	0.500	0.000	0.000

高温高压下的
晶体结构相变

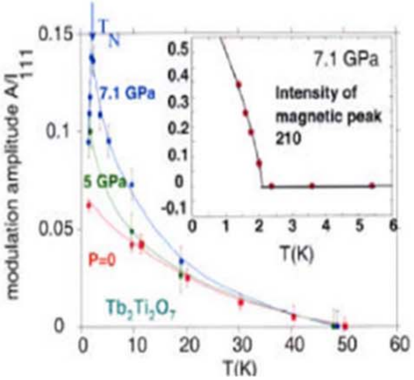
原子分子结构
微观与宏观

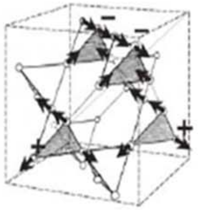

Understanding the micro-to-macro relations

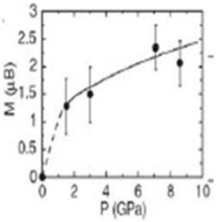


磁矩与相变

原子位置与热运动





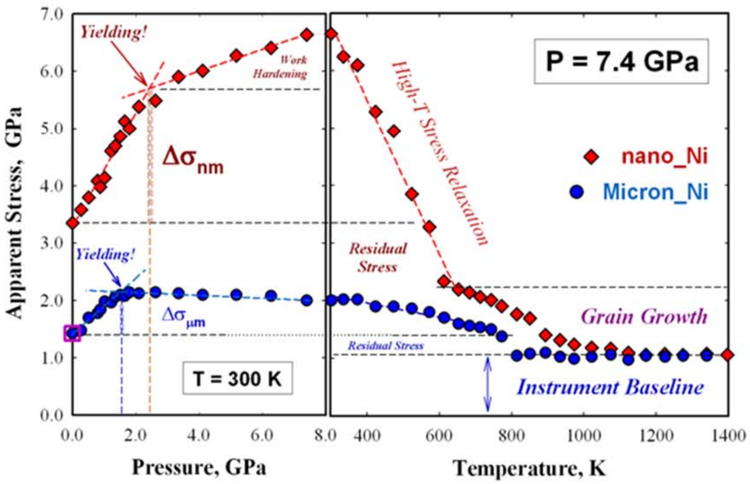


高温高压下的
纳米力学性质

高温高压下的
磁学性质变化

高温高压下的
岩石形变力学

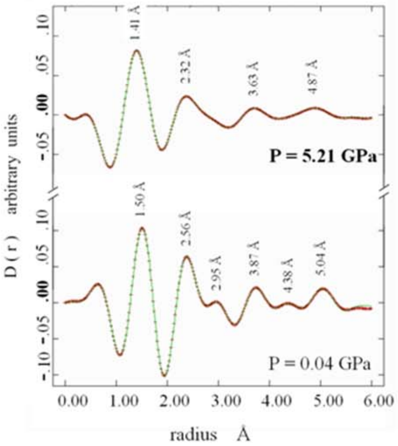
High *P-T* Constitutive Property of Nano-/Micron- Nickel Polycrystallines



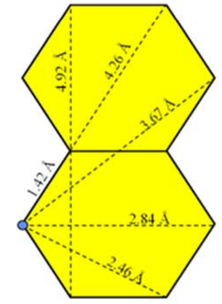
纳米材料
塑性力学
（屈服与形变）

高温高压下的
相邻分布函数

Pair Distribution Function (PDF) study indicates that amorphous carbon black under high-pressure becomes graphitized



To understand aging and fatigue of rubber at extreme conditions



Hexagonal Graphite Ring