Energy Frontier Research Center

Energy Frontier Research in Extreme Environment (EFree)

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Director of EFree

Carnegie Institution of Washington

NNSA SSGF Conference

July 22, 2011, Arlington, VA

OUTLINE

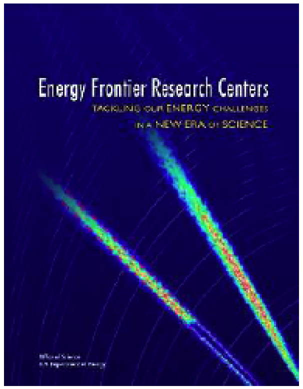
- DOE-EFRC
- Introduction of EFree
- Extreme properties:
  Nano XRD
  Superconducting Si_2H_6
  Highest H compound
  Highest Tc element – Ca
  Lowest melting T – Li
  Bi2223 superconductor
  Widest bandgap – He
- Recoverable examples:
  GaAs
  PIA of nano Y_2O_3
  Mesoporous diamond
  Ce_3Al alloy
  Perfect glass – long-range topological order
  Mesoporous diamonds
  Mesoporous quartz
- Summary

The Size of the Energy Challenge

U.S. DEPARTMENT OF ENERGY | Office of Science

Energy Frontier Research Centers

Tackling Our Energy Challenges in a New Era of Science



"To harness the most basic and advanced discovery research in a concerted effort to establish the scientific foundation for a fundamentally new U.S. energy economy. The outcome will decisively enhance U.S. energy security and protect the global environment in the century ahead."

Key characteristics:

- **To engage the talents of the nation's researchers for the broad energy sciences**
- **To accelerate the scientific breakthroughs needed to create advanced energy technologies for the 21st century**
- **To pursue the fundamental understanding necessary to meet the global need for abundant, clean, and economical energy**

Be Bold, Imaginative, and Impactful!

Basic and Applied Research Integration

How Nature Works ··· Design and Control ··· Technologies for the 21st Century

Grand Challenges	Discovery and Use-Inspired Basic Research		Applied Research	Technology Maturation & Deployment
How nature works	*Materials properties and chemical functionalities by design*			

Grand Challenges — *How nature works*

- Controlling materials processes at the level of quantum behavior of electrons
- Atom- and energy-efficient syntheses of new forms of matter with tailored properties
- Emergent properties from complex correlations of atomic and electronic constituents
- Man-made nanoscale objects with capabilities rivaling those of living things
- Controlling matter very far away from equilibrium

Discovery and Use-Inspired Basic Research — *Materials properties and chemical functionalities by design*

- Basic research for fundamental new understanding on materials or systems that may revolutionize or transform today's energy technologies
- Development of new tools, techniques, and facilities, including those for the scattering sciences and for advanced modeling and computation
- Basic research, often with the goal of addressing showstoppers on real-world applications in the energy technologies

Applied Research

- Research with the goal of meeting *technical milestones*, with emphasis on the development, performance, cost reduction, and durability of materials and components or on efficient processes
- Proof of technology concepts

Technology Maturation & Deployment

- Scale-up research
- At-scale demonstration
- Cost reduction
- Prototyping
- Manufacturing R&D
- Deployment support

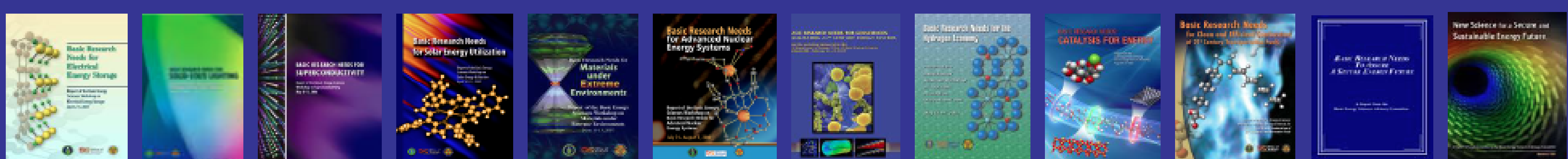
BESAC & BES Basic Research Needs Workshops

BESAC Grand Challenges Panel

DOE Technology Office/Industry Roadmaps

EFree

EFRC



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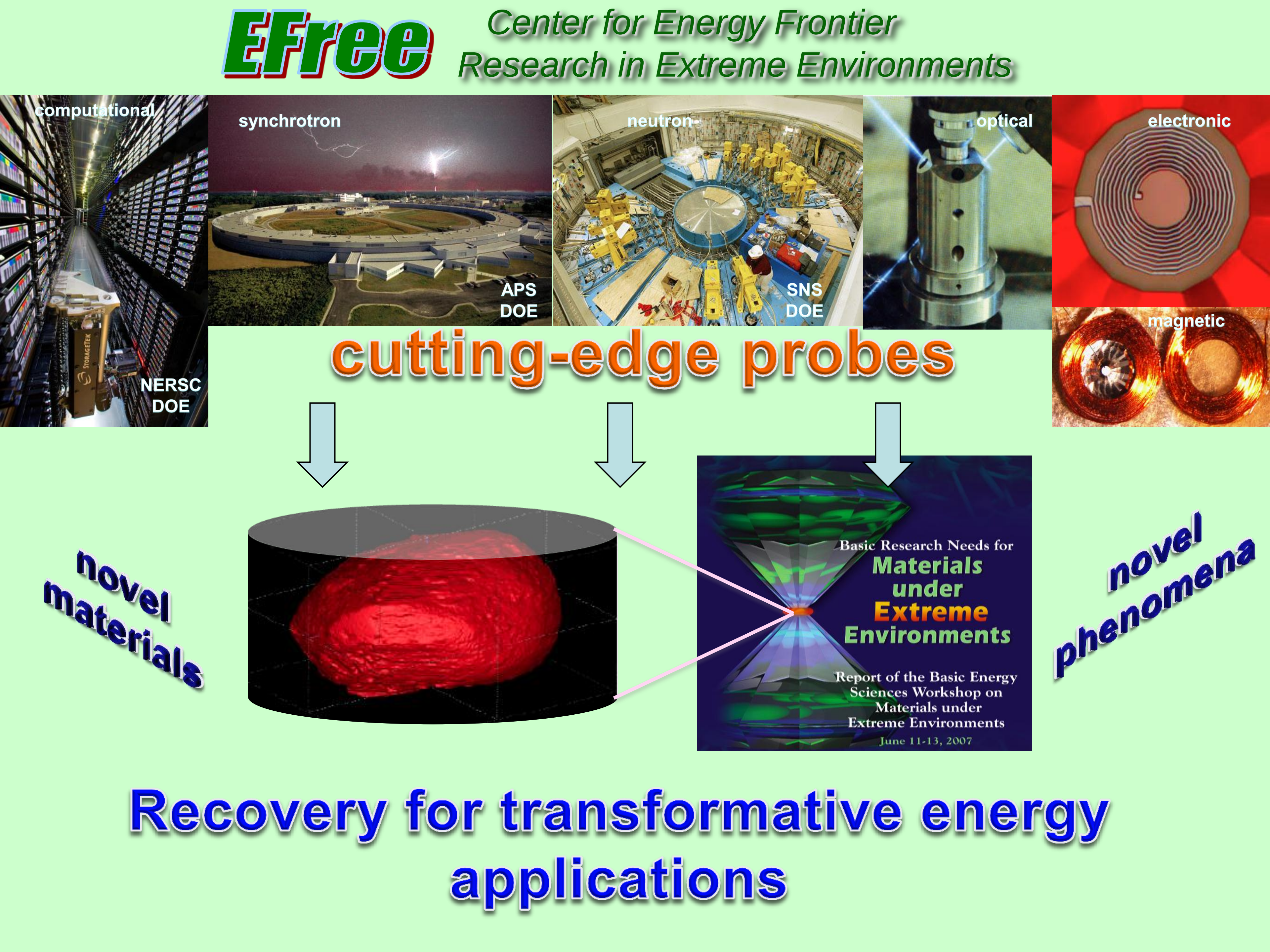
Energy Frontier Research in Extreme Environments

Why high pressure?

- *nearly unexplored*
- *> ten times unknown materials*
- *novel physics and chemistry*
- *extremely favorable properties for energy applications*

EFRC

CARNEGIE INSTITUTION FOR SCIENCE


EFree
Center for Energy Frontier
Research in Extreme Environments
computational
NERSC
DOE
synchrotron
APS
DOE
neutron
SNS
DOE
optical
electronic
magnetic
cutting-edge probes
novel materials
Basic Research Needs for
Materials under Extreme Environments
Report of the Basic Energy Sciences Workshop on Materials under Extreme Environments
June 11-13, 2007
novel phenomena
Recovery for transformative energy applications

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Energy Frontier Research in Extreme Environments

How is EFree distinct from other high-pressure programs?

- *unprecedented team works for the energy cause*
- *unprecedented advances of the enabling high-pressure technology*

EFRC

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Design of Anvils and DAC

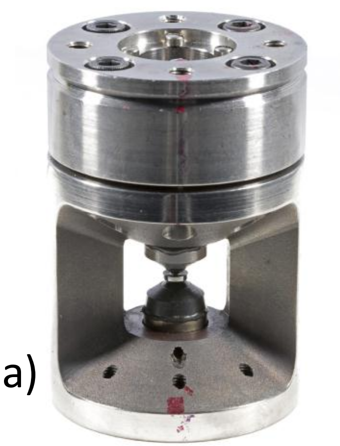
Reini Boehler

Goals:

Higher pressures
High-low temperatures
Larger sample volume
Probing Accessibility
Easier operation

Equipment

Eximer laser and FIB to shape diamond anvils
CVD diamond anvils
Radically different designs: plate DAC, cross DAC

a) 

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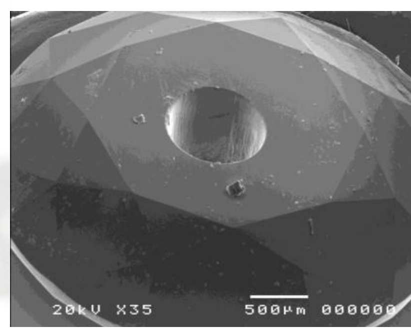

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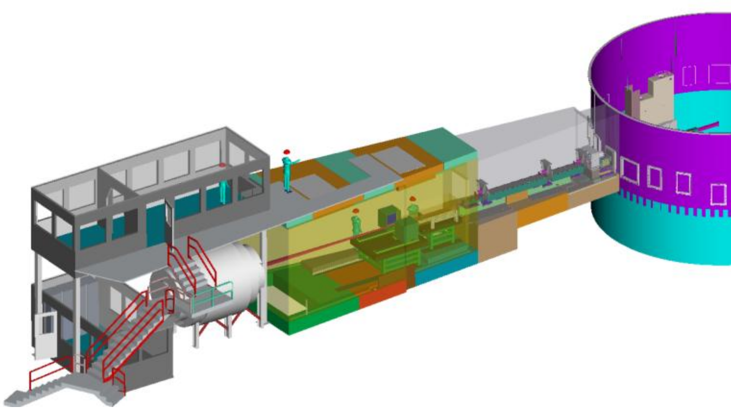
Neutron power for EFree science

Neutrons
M. Guthrie

Enabled HP research on:
Hydrogen rich materials
Superconductors
Magnetic ordering
Amorphous structures
Light elements

Establishing HP-IDT at SNS-JIN
EFree is a resident user at SNS,
with a staff and PDs/students
SNS matches with full equipment
and 50-50 PD/student



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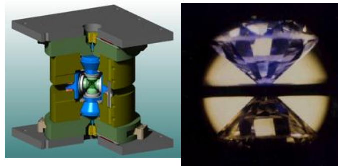
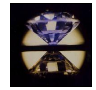
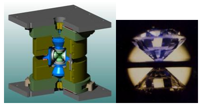
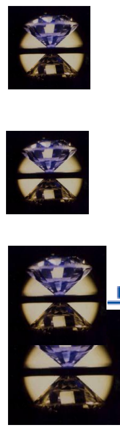
Synchrotron for HP

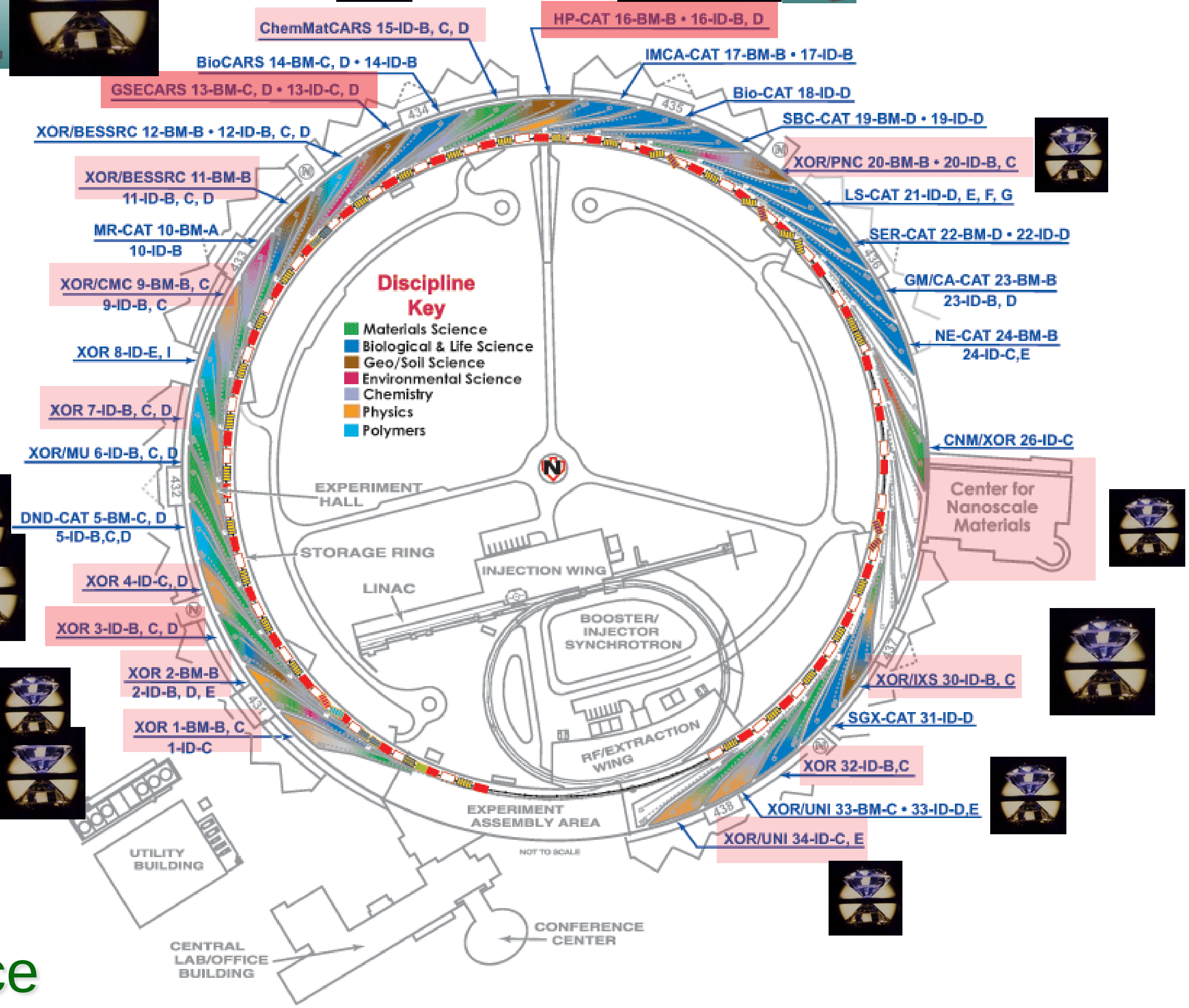
Synchrotron Radiation











HP Beamlines
-HPCAT
Guoyin Shen
-GSECARS
are two most Productive sectors

HP Experiments at more than 13 other specialized sectors

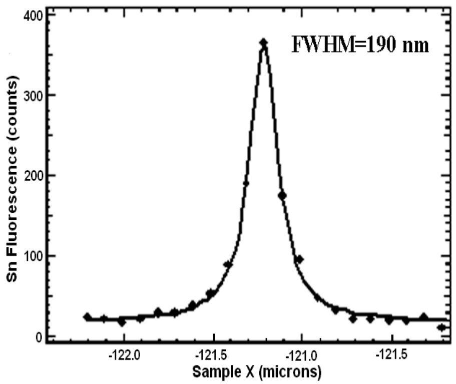
EFree supported HPSynch enables novel HP-SR science

Wenge Yang

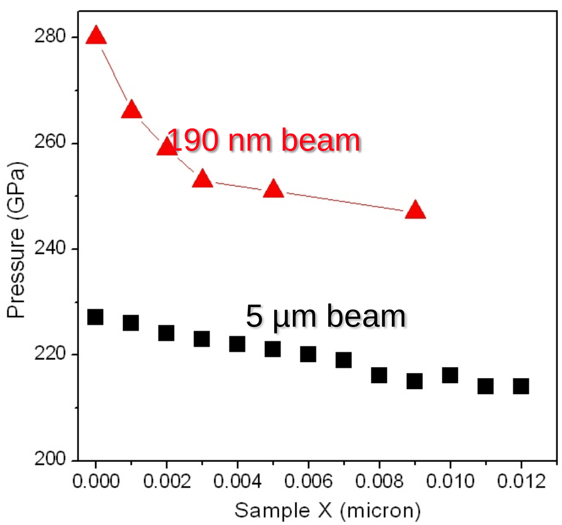
EFree

Using 200 nm focused x-ray beam at 2-ID and 34-ID

Lin Wang et al., *PNAS* *107,* 6140 (2010)

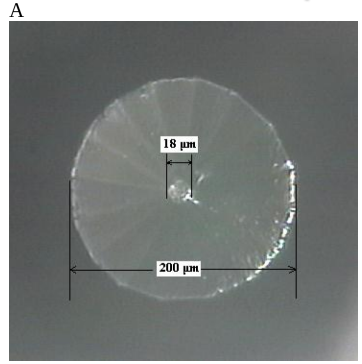


Observe 20 GPa/µm *P* gradiant & peak-pressure in 1-µm area

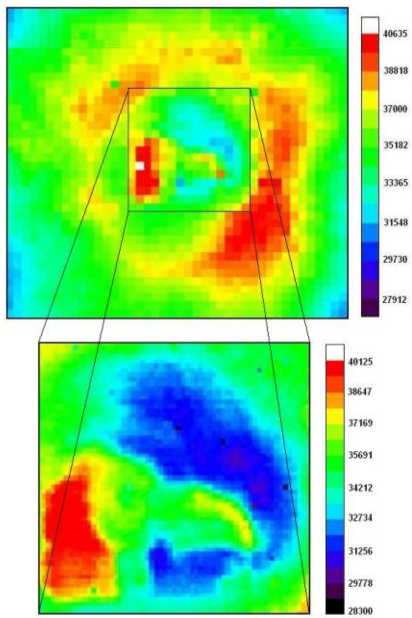


Separate submicron Pt, Re, Fe samples

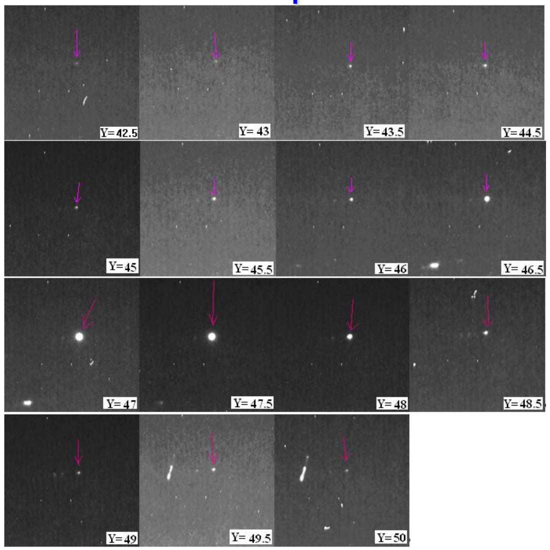
A

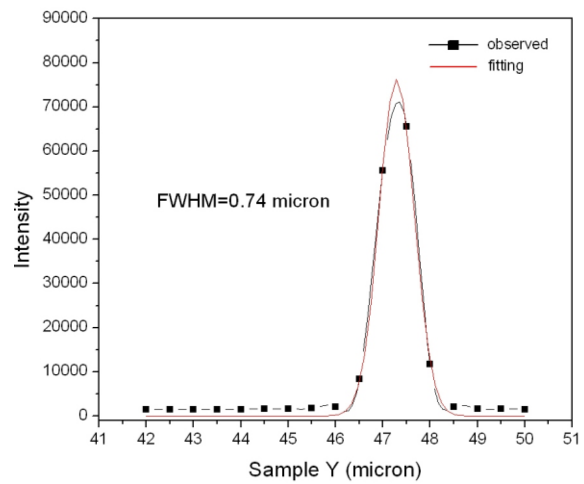


B

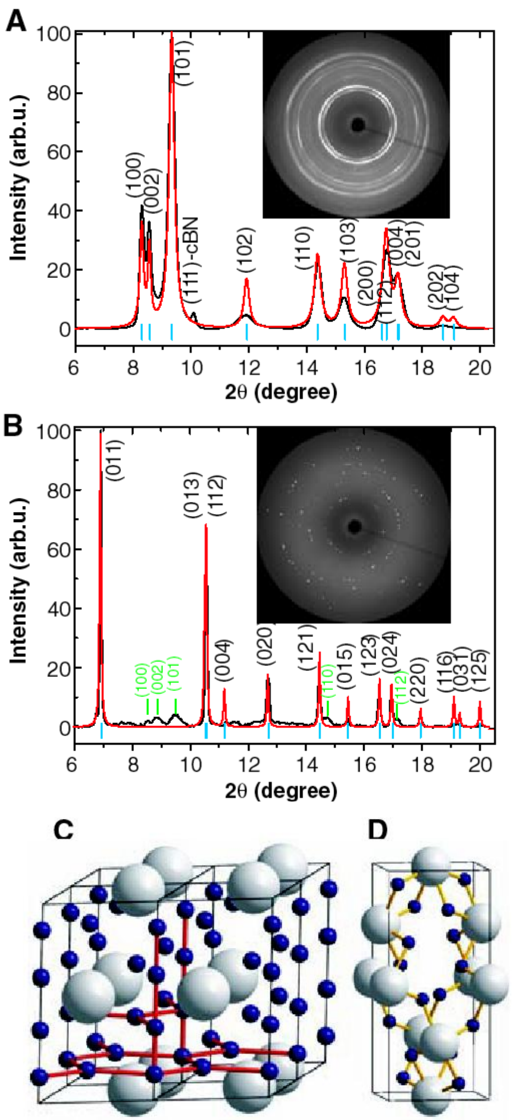


Conduct single-crystal XRD on submicron powder





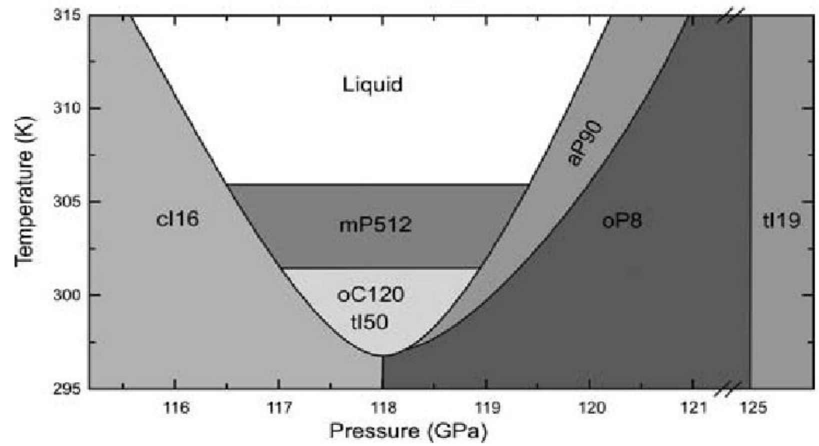
The need of submicron x-ray beam



SiH$_4$

Eremets et al., Suerconductivity in silane, *Science* ***319***, 1506 (2008)

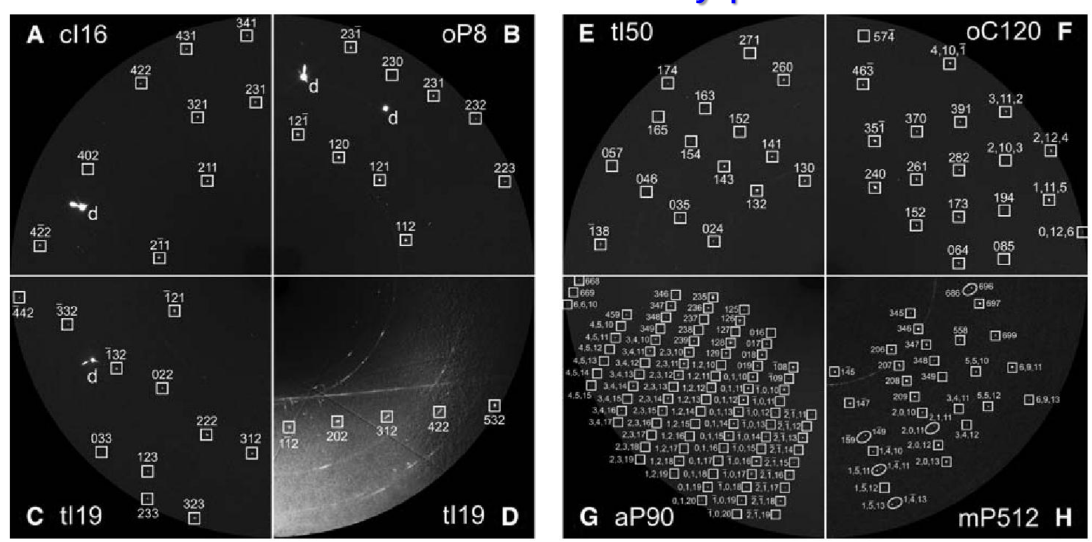
Most HP structures were determined with μm-size powder XRD; assignments were questionable.



Gregoryanz et al., Structural diversity of sodium *Science* ***320***, 1054 (2008)

Na

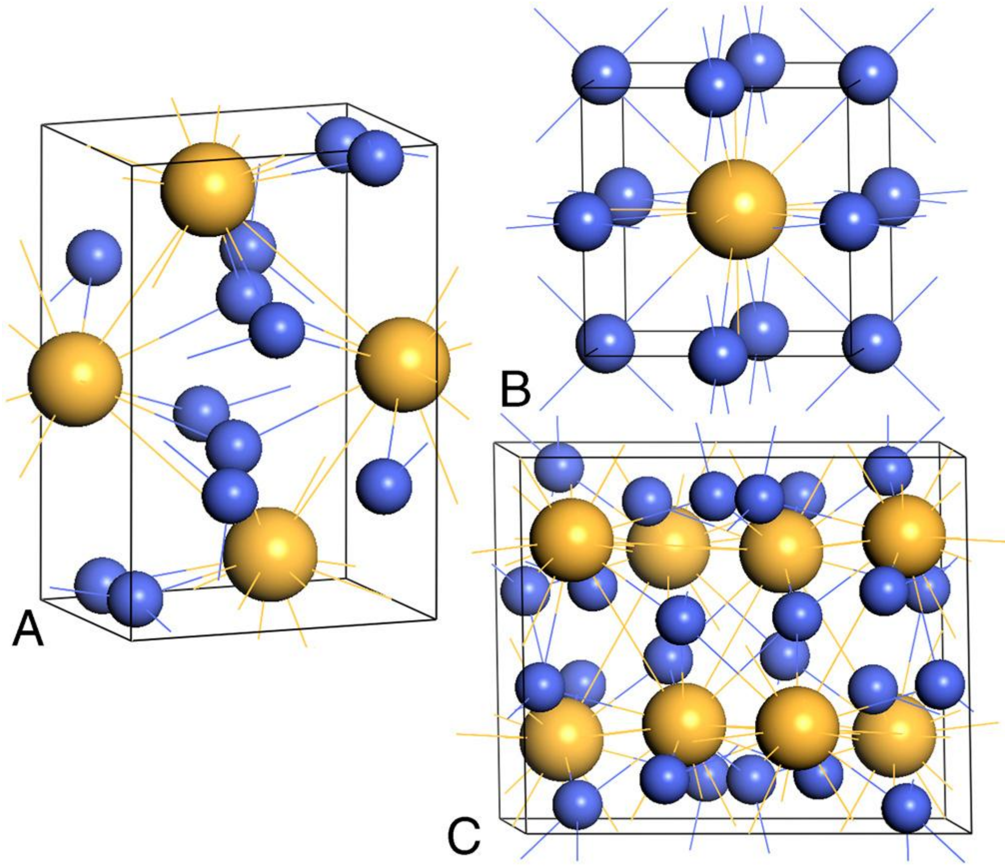
Single-crystal XRD gives definitive answer, but requires crystals larger than the x-ray probe.



EFree

HP disilane (Si_2H_6) has Tc >100K?

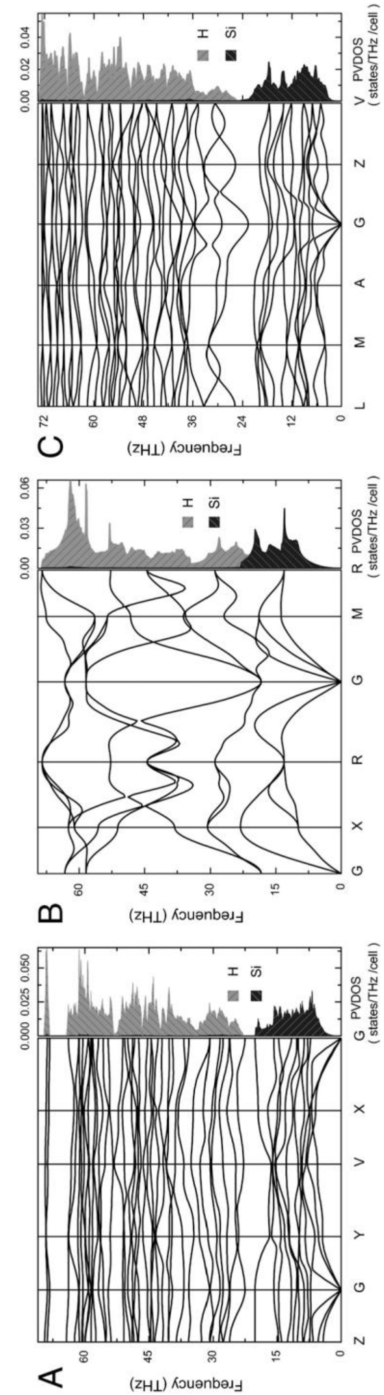
Xilian Jin, Xing Meng, Zhi He, Yanming Ma, Bingbing Liu, Tian Cui, Guangtian Zou, and Ho-kwang Mao, *Proc. Nat. Acad. Sci. USA 107,* 9969−9973 (2010)



$Pm\bar{3}m$
275 GPa
Tc 134K

C2/c
300 GPa
Tc 34 K

$P\bar{1}$
175 GPa
Tc 65-80 K

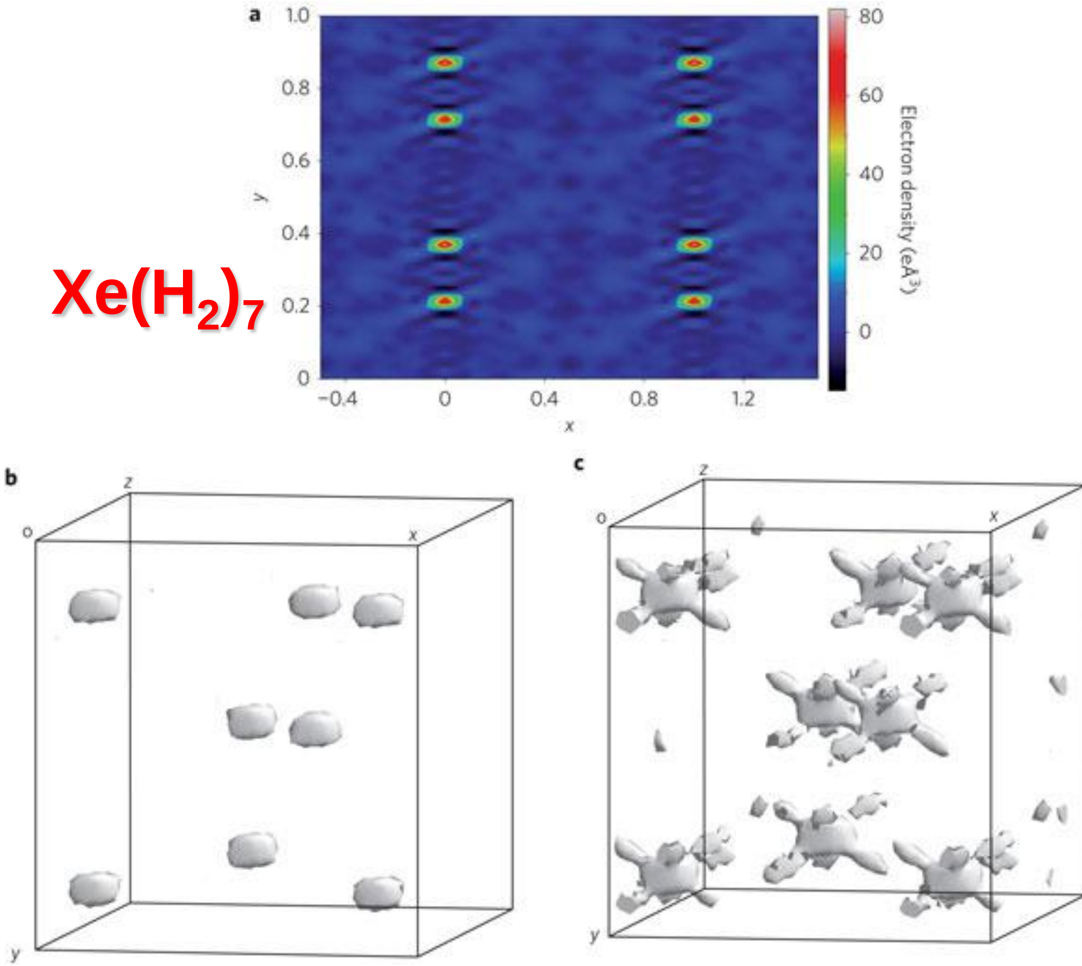


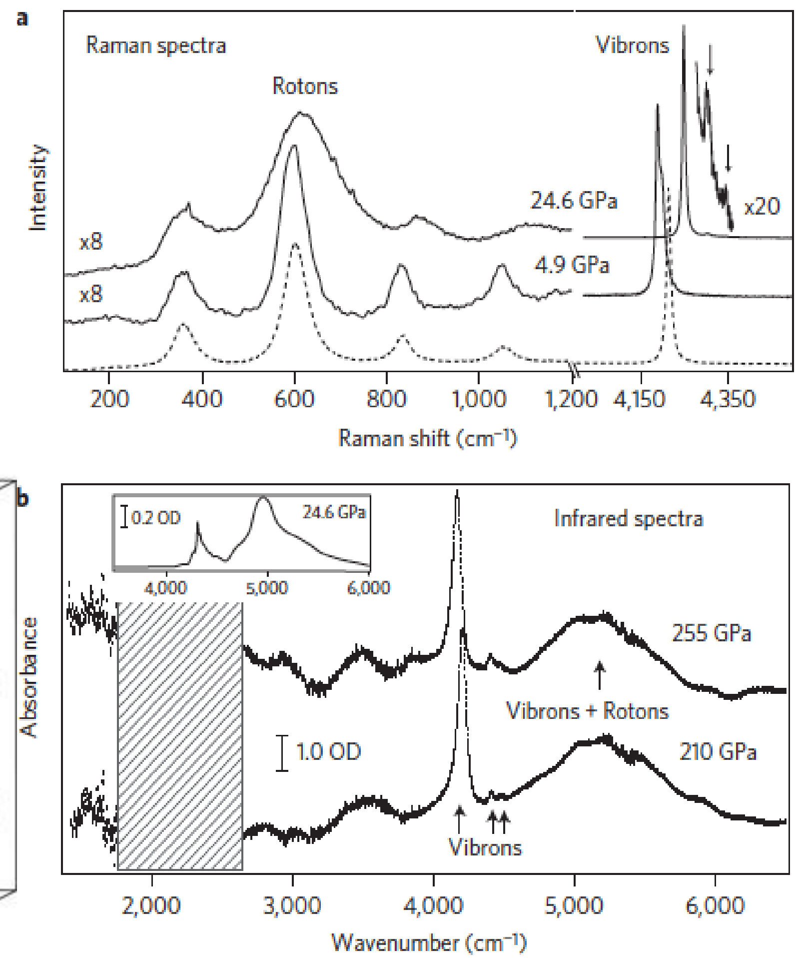
EFree

A HP compound with the highest H-content

Maddury Somayazulu, Przemyslaw Dera, Alexander F. Goncharov, Stephen A. Gramsch, Peter Liermann, Wenge Yang, Zhenxian Liu, Ho-kwang Mao and Russell J. Hemley, *Nature Chemistry 2,* 50-53 (2010)

$Xe(H_2)_7$

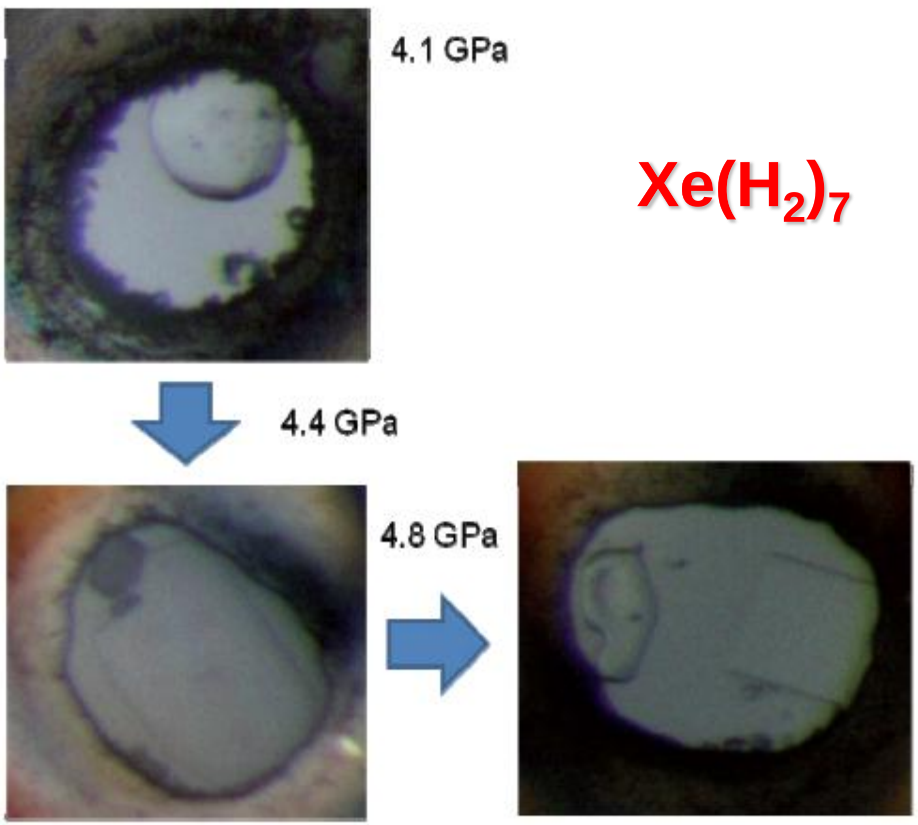




EFree

A HP compound has the highest H-content (14:1)

Maddury Somayazulu, Przemyslaw Dera, Alexander F. Goncharov, Stephen A. Gramsch, Peter Liermann, Wenge Yang, Zhenxian Liu, Ho-kwang Mao and Russell J. Hemley, *Nature Chemistry 2,* 50-53 (2010)



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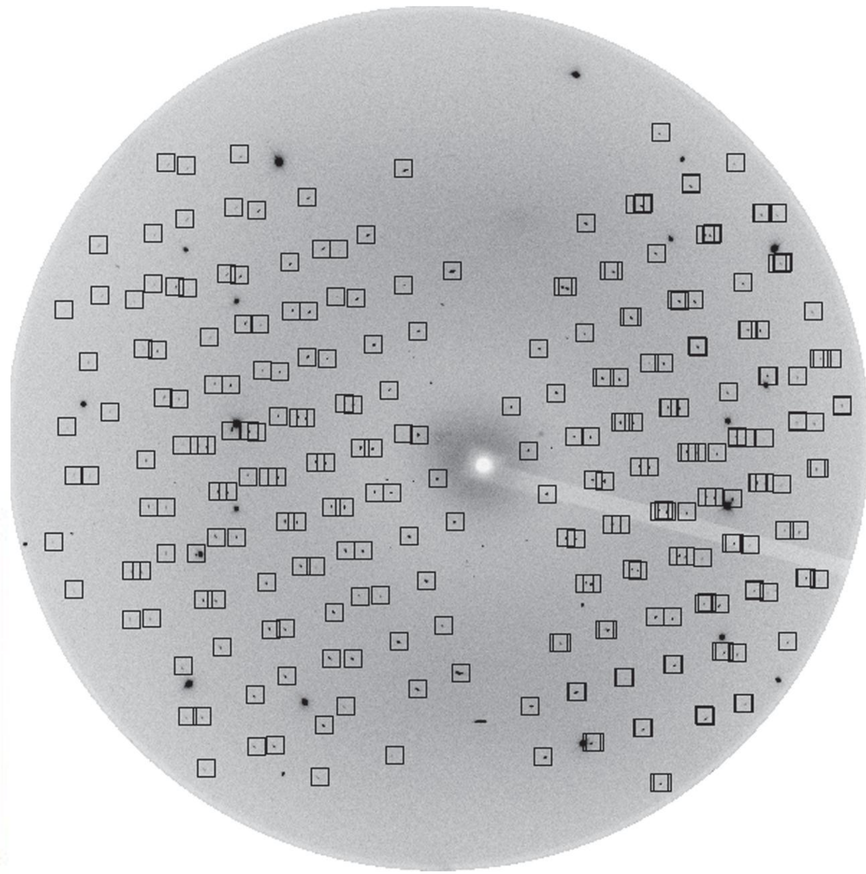
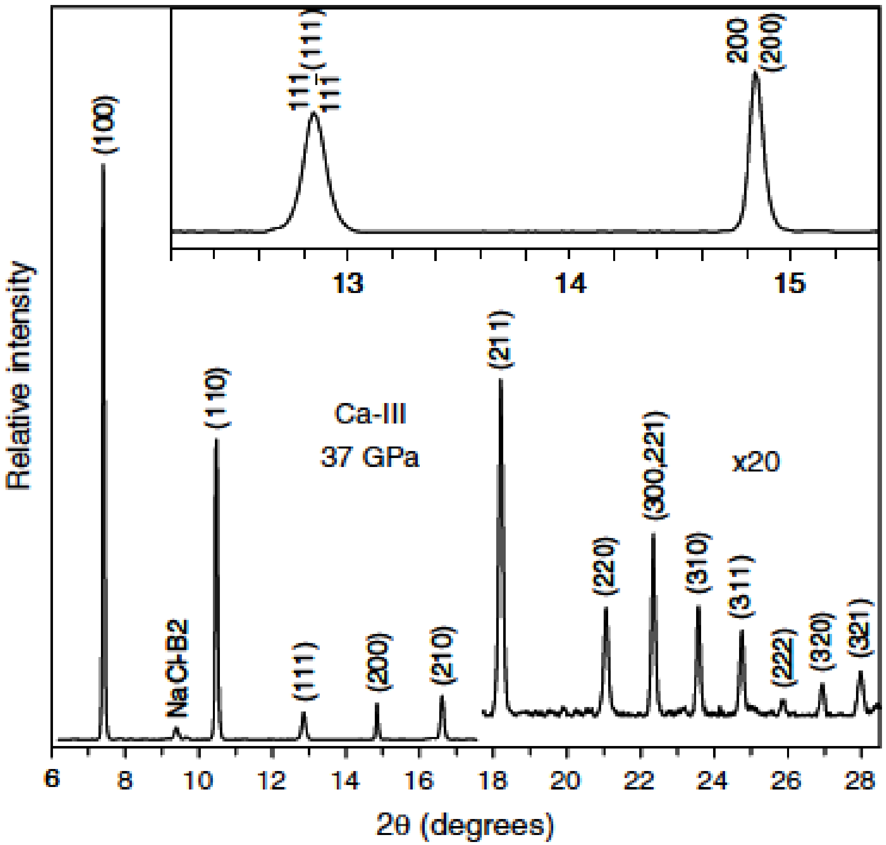
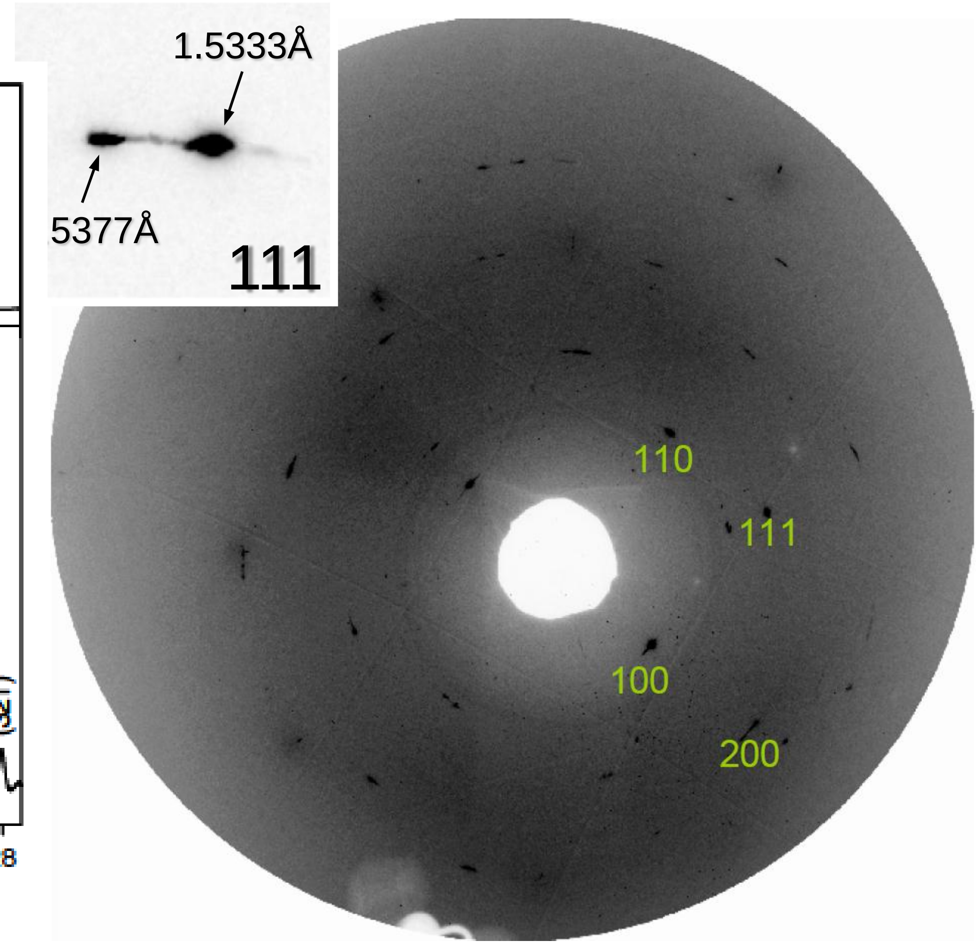


EFree

Simple cubic calcium above 30 GPa

Wendy L. Mao, Lin Wang Yang Ding, Wenge Yang, Wenjun Liu, Duck Young Kim, Wei Luo, Rajeev Ahuja, Yue Meng, Stas Sinogeikin, Jinfu Shu, & Ho-kwang Mao, *Proc. Nat. Acad. Sci. USA 107,* 9965 (2010)

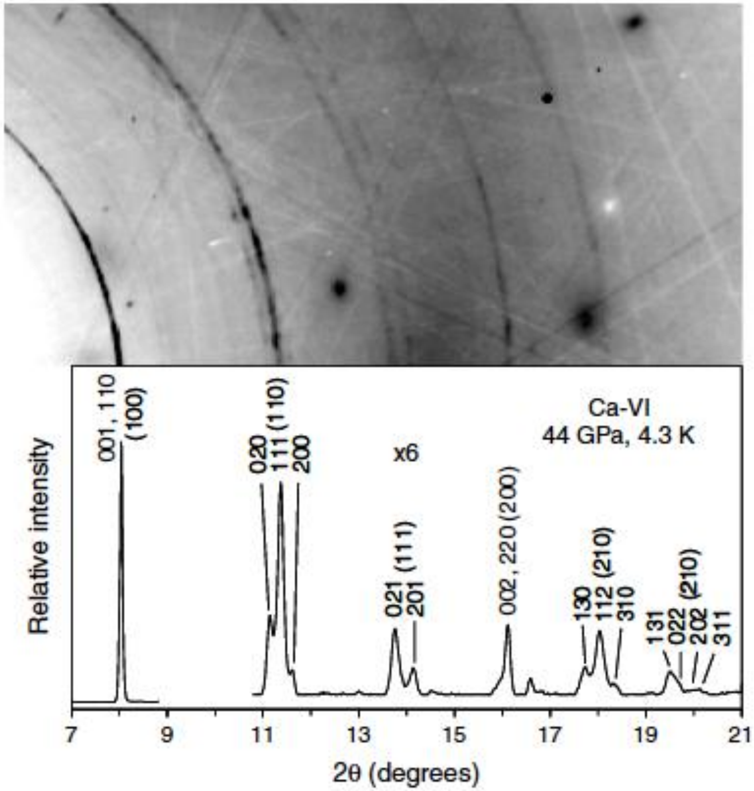


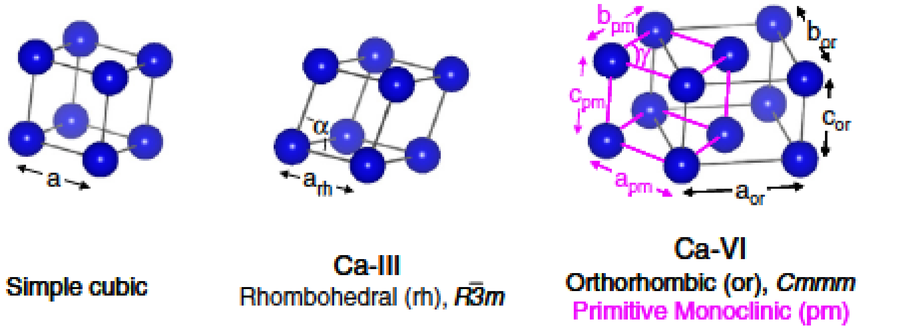


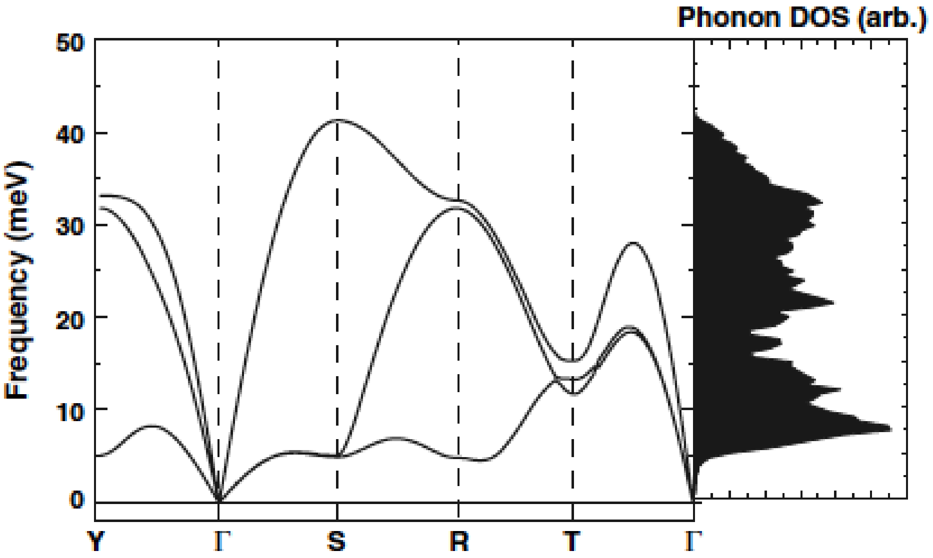
Picking sub-µm single crystal out of the polycrystalline XRD reveals rhombohedral distortion

EFree HP calcium is the element with highest Tc=25K

Wendy L. Mao, Lin Wang, Yang Ding, Wenge Yang, Wenjun Liu, Duck Young Kim, Wei Luo, Rajeev Ahuja, Yue Meng, Stas Sinogeikin, Jinfu Shu, & Ho-kwang Mao, *Proc. Nat. Acad. Sci. USA 107,* 9965 (2010)



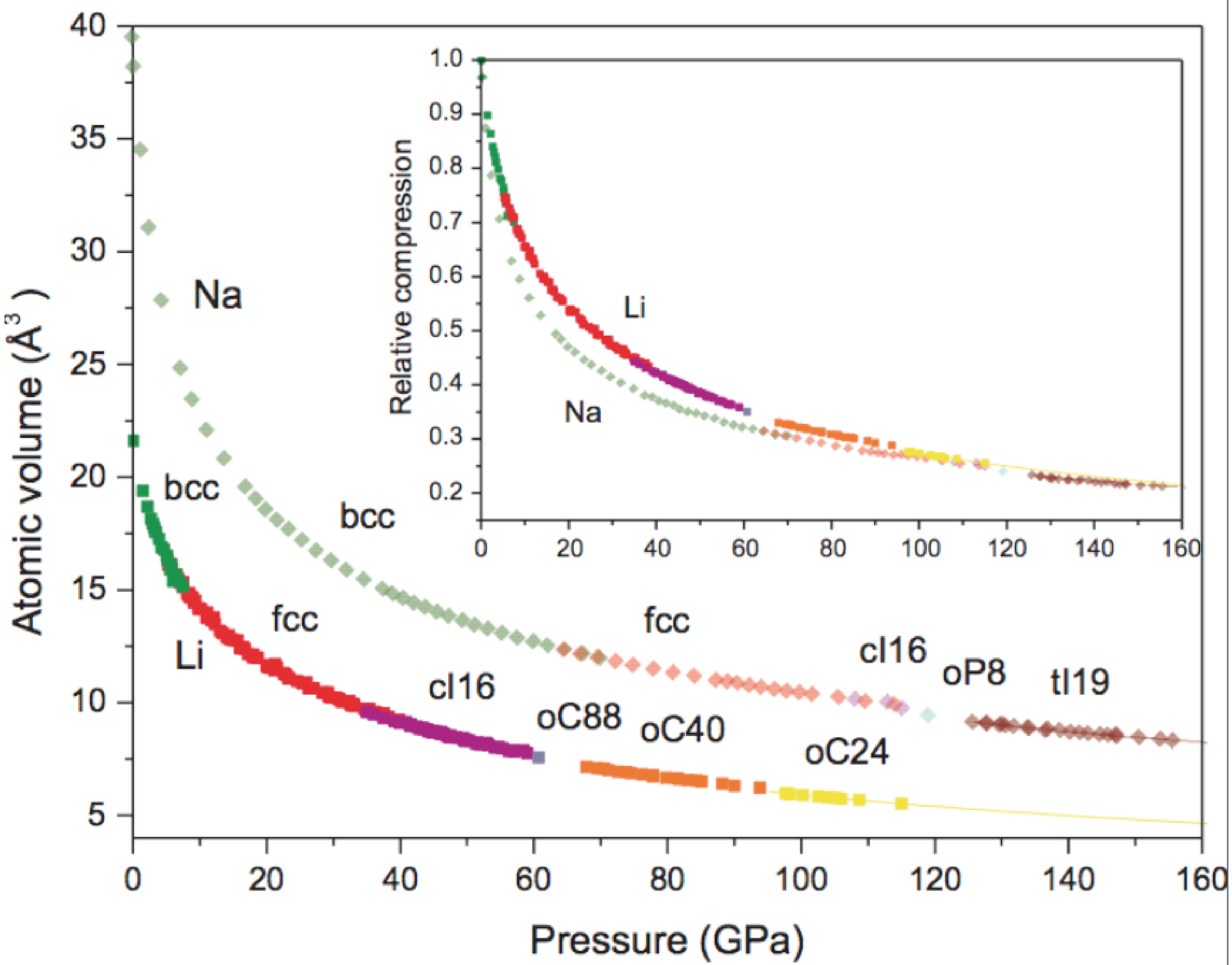




At low T, the superconducting Ca further distorted to orthorhombic *Cmmm*

EFree Cold melting and solid structures of dense lithium

Christophe L. Guillaume, Eugene Gregoryanz, Olga Degtyareva, Malcolm I. McMahon, Shaun Evans, Michael Hanfland, Malcolm Guthrie, Stas V. Sinogeikin, & H-K. Mao, *Nature Physics January 9,* 2011



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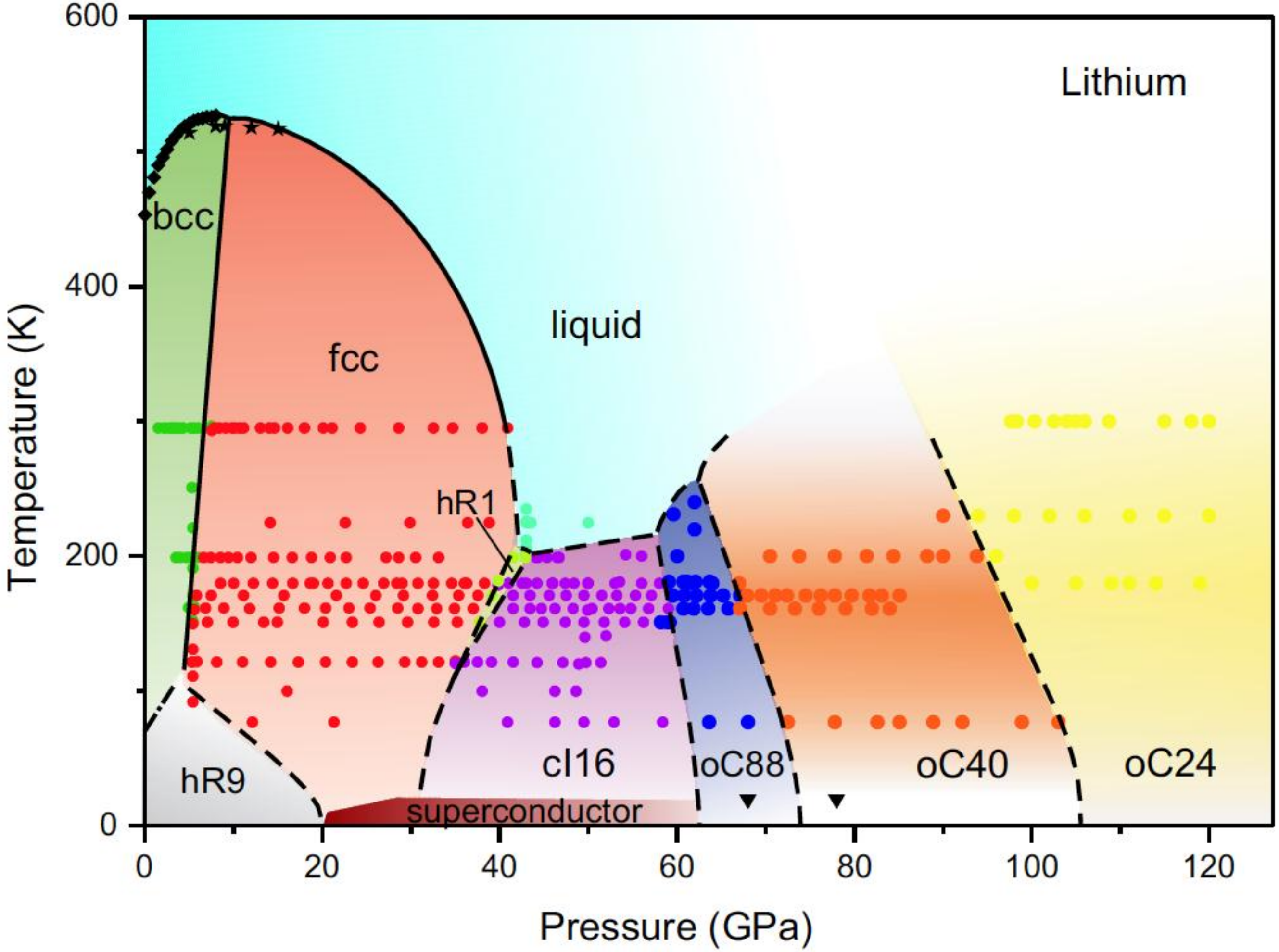
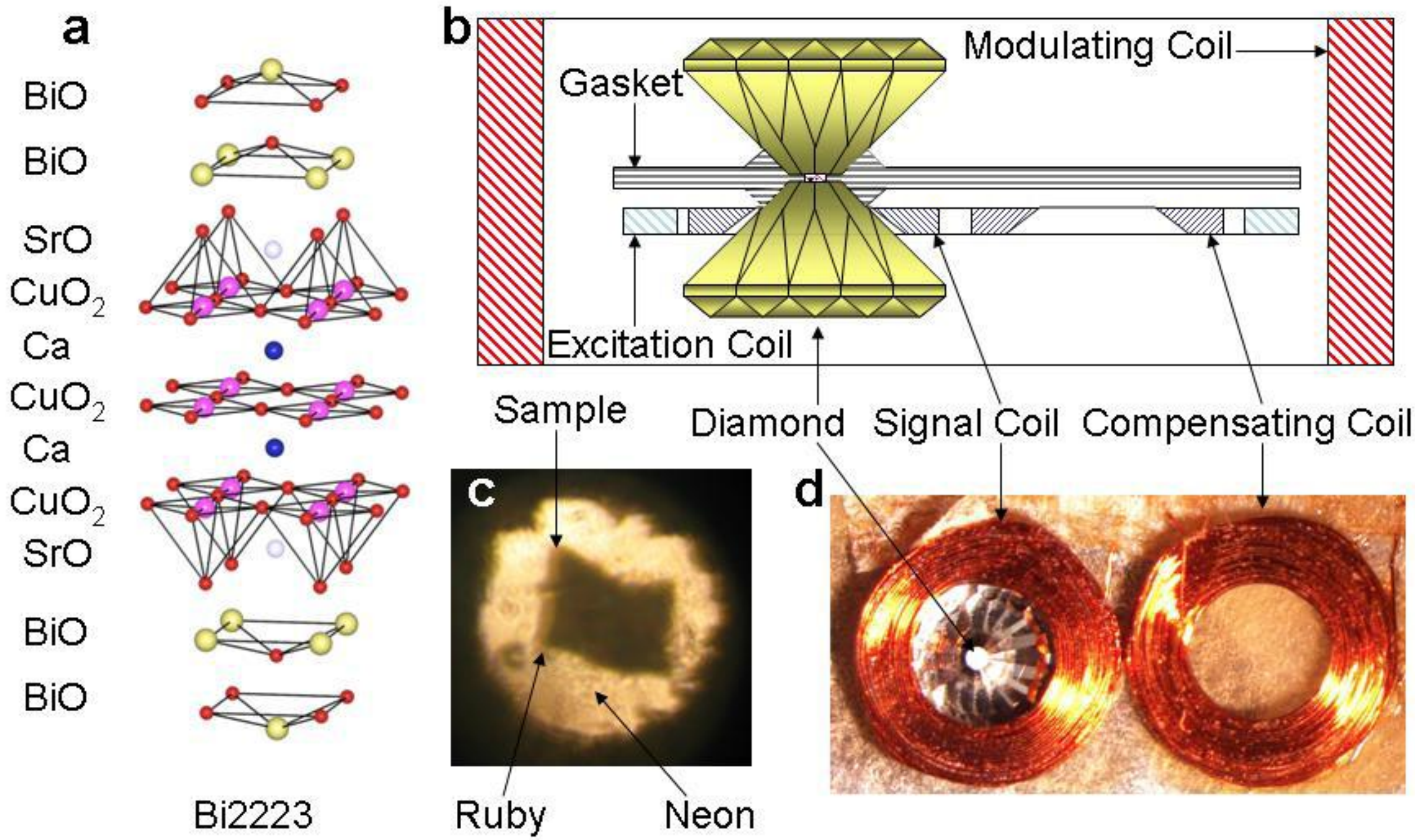


EFree

Enhancement of Superconductivity by Pressure-Driven Competition in Electronic Order

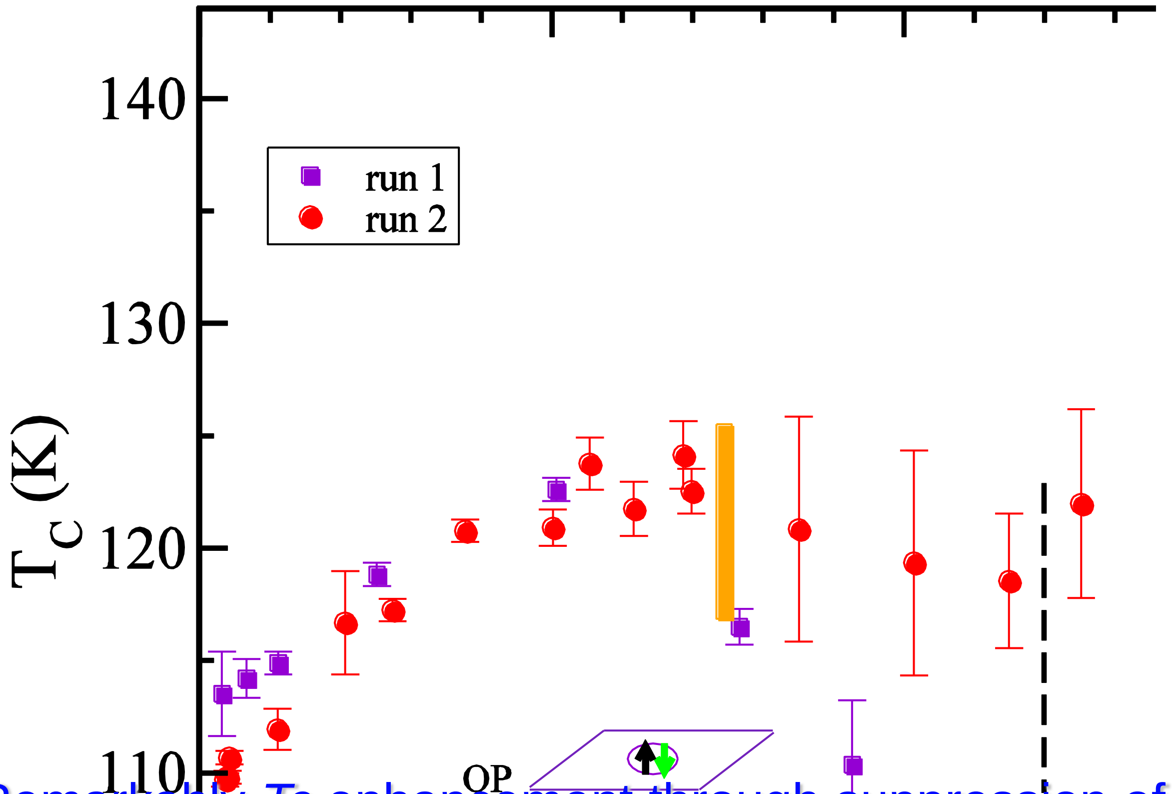
Xiao-Jia Chen, Viktor V. Struzhkin, Yong Yu, Alexander F. Goncharov, Cheng-Tian Lin, Ho-kwang Mao & Russell J. Hemley, *Nature 466,* 950 (2010)

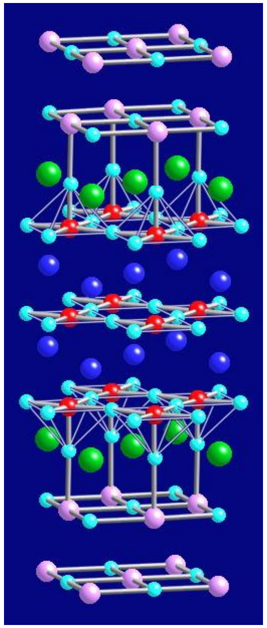


$Bi_2Sr_2Ca_2Cu_3O_{10+\delta}$

EFree

Enhancement of Superconductivity by Pressure-Driven Competition in Electronic Order



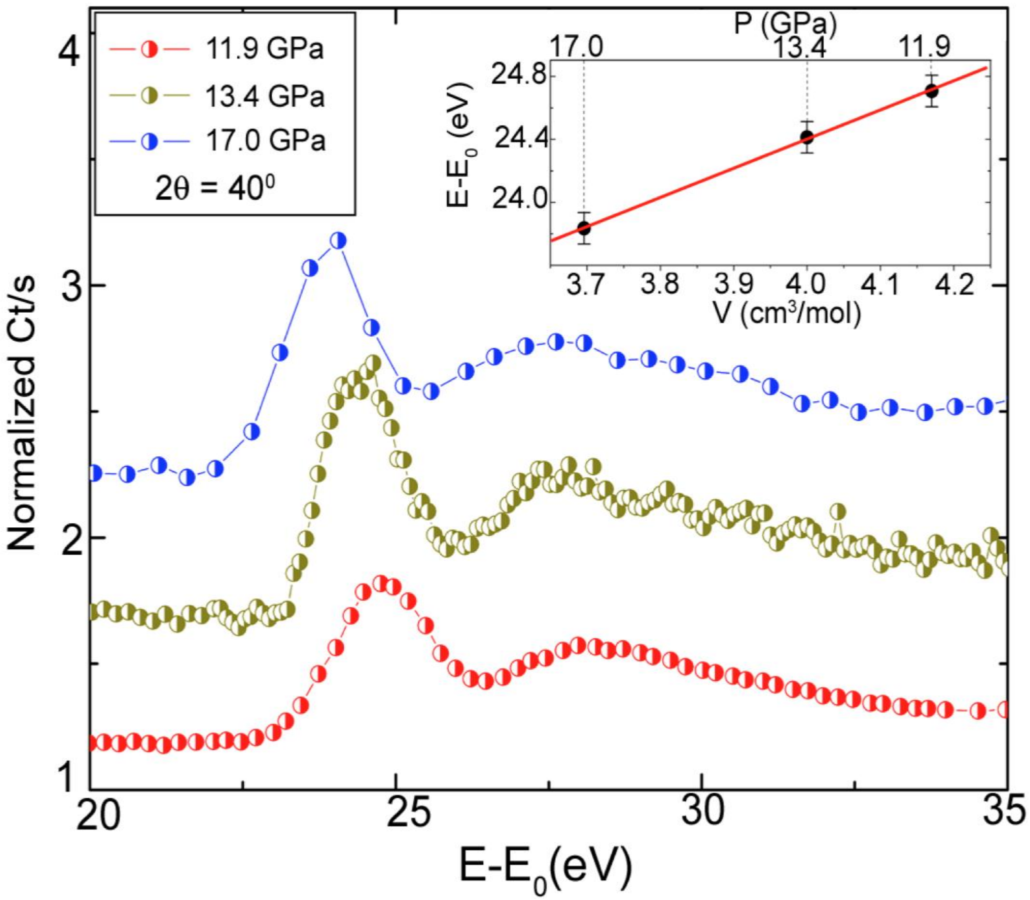


Remarkably *Tc* enhancement through suppression of AFM in the inner CuO_2 plane and optimization of competing pairing and phase ordering energy scales.

Xiao-Jia Chen, Viktor V. Struzhkin, Yong Yu, Alexander F. Goncharov, Cheng-Tian Lin, Ho-kwang Mao & Russell J. Hemley, *Nature 466,* 950 (2010)

Electronic Dynamics of Crystalline ^{4}He at High-P

Ho Kwang Mao, Eric L. Shirley, Yang Ding, Peter Eng, Yong Q. Ca, Paul Chow, Yuming Xiao, Jinfu Shu, Russell J. Hemley, Chichang Kao, & Wendy L. Mao, *PRL 105,* 186404 (2010)



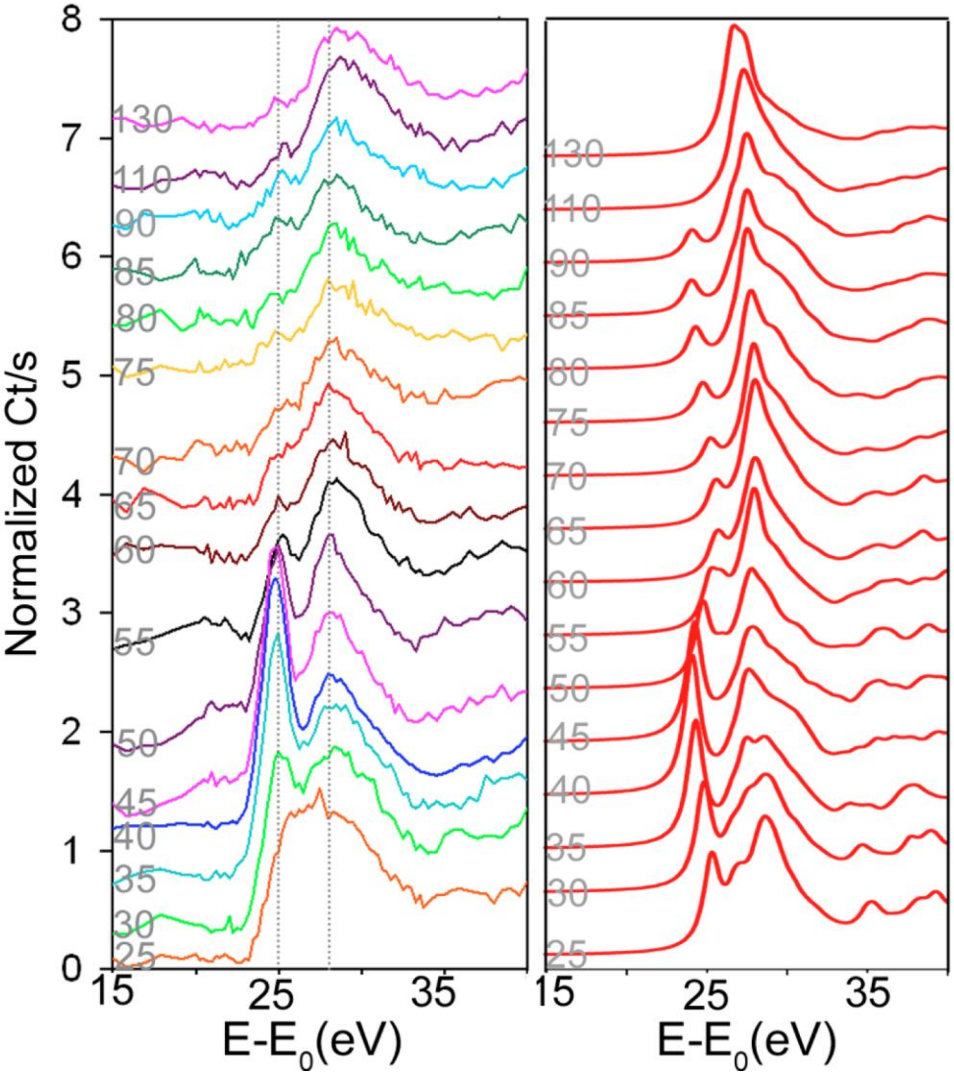
- Helium has the widest electronic band gap and highest metallization *P*
- "Optical spectrum": cut-off edge, exciton, multiple excitations & continuum are now accessible by inelastic X-ray scattering (IXS)
- 11.9 GPa (GSECARS)
  13.4 GPa (BL12XU, Taiwan Beamline, SPring-8)
  17 GPa (HPCAT).

Γ-M Dispersion of single-crystal He electronic excitation

Mao et al, *Phys. Rev. Lett. 105*, 186404 (2010)

11.9GPa

IXS from GSECARS

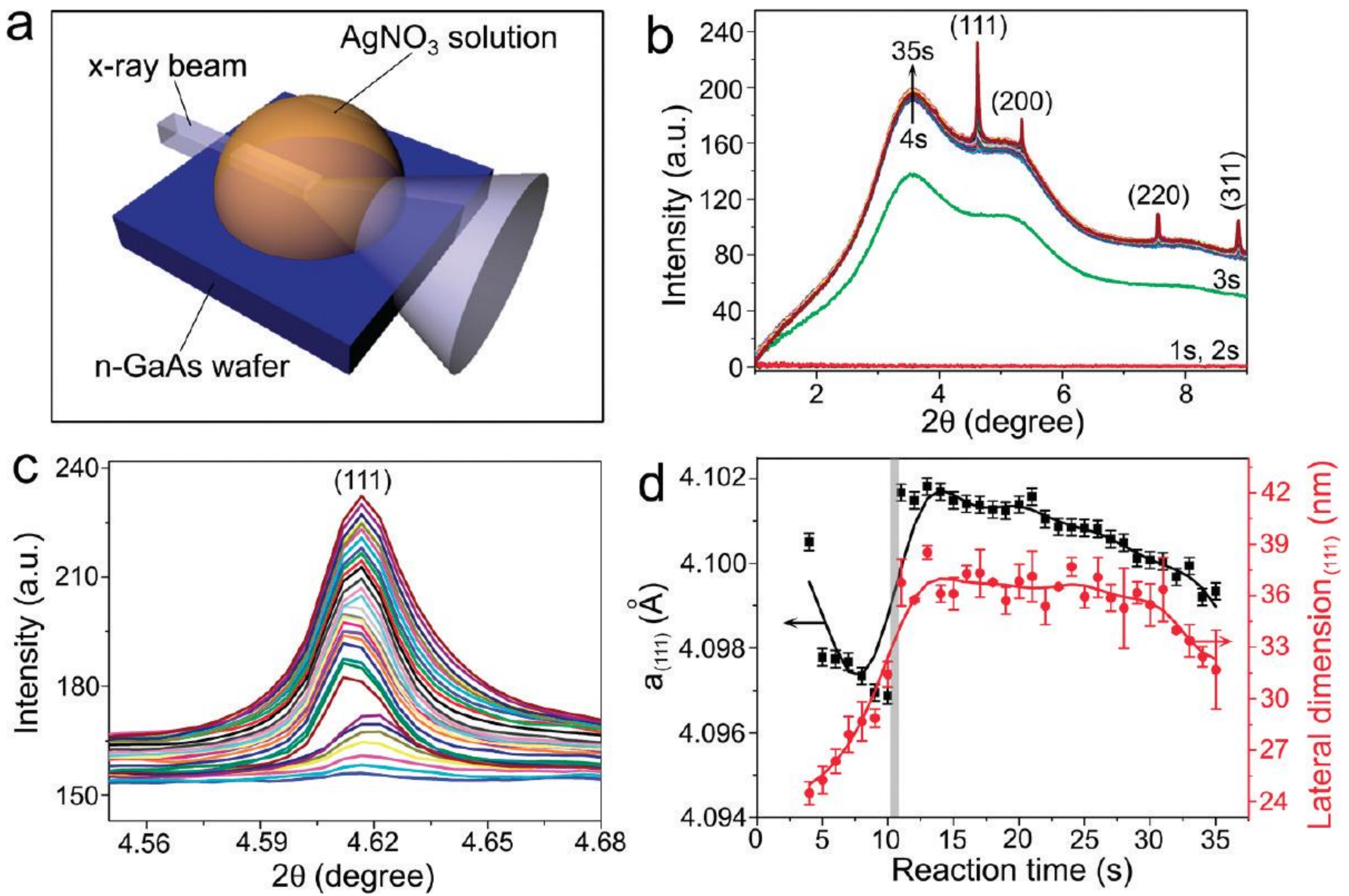


Theory
(Eric Shirley)

EFree

Watching Ag nano particle growth on GaAs

Yugang Sun, Yang Ren, Dean R. Haeffner, Jonathan D. Almer, Lin Wang, Wenge Yang, and Tu T. Truong, *Nano Lett. 10,* 3747-3753 (2010)



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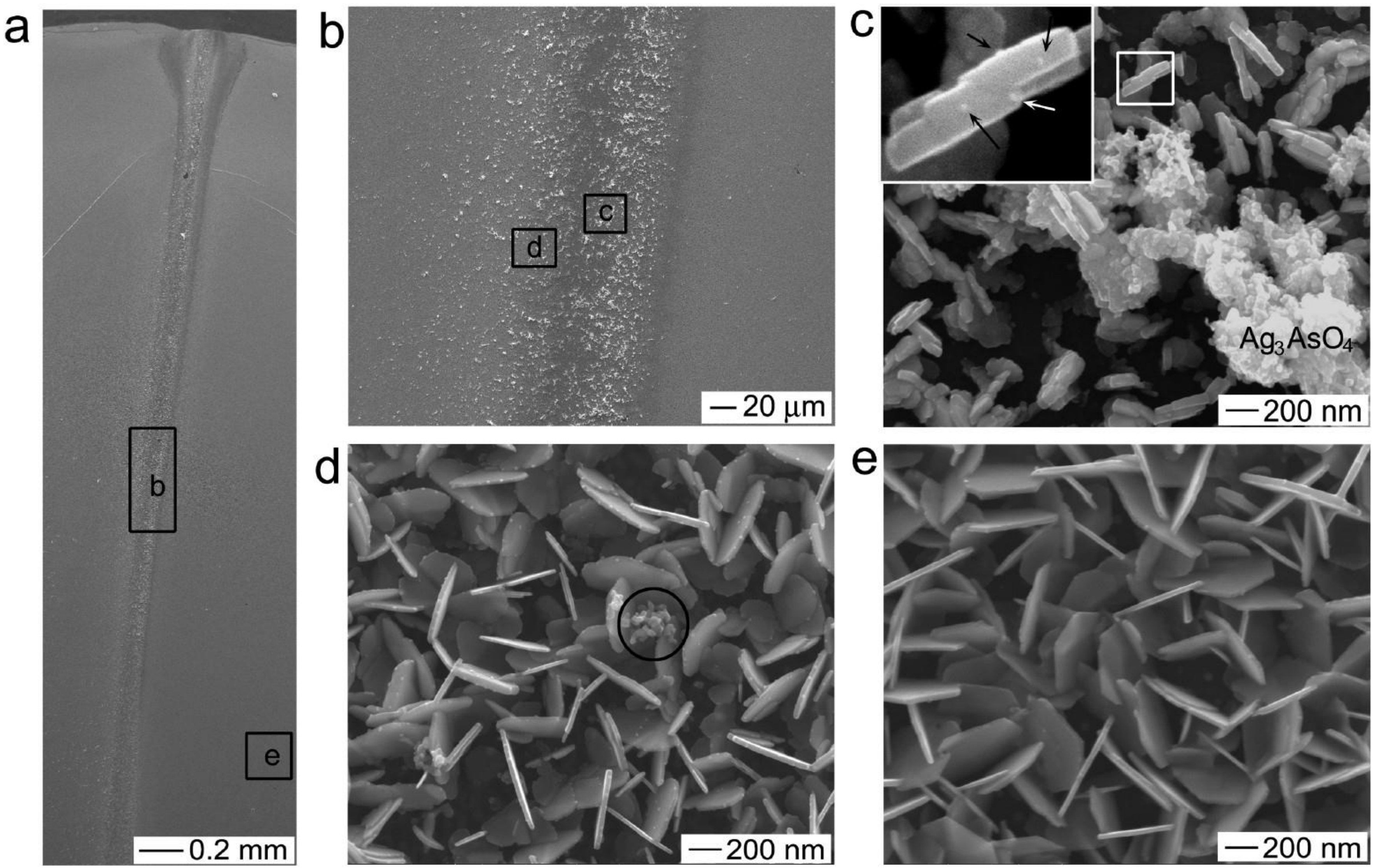
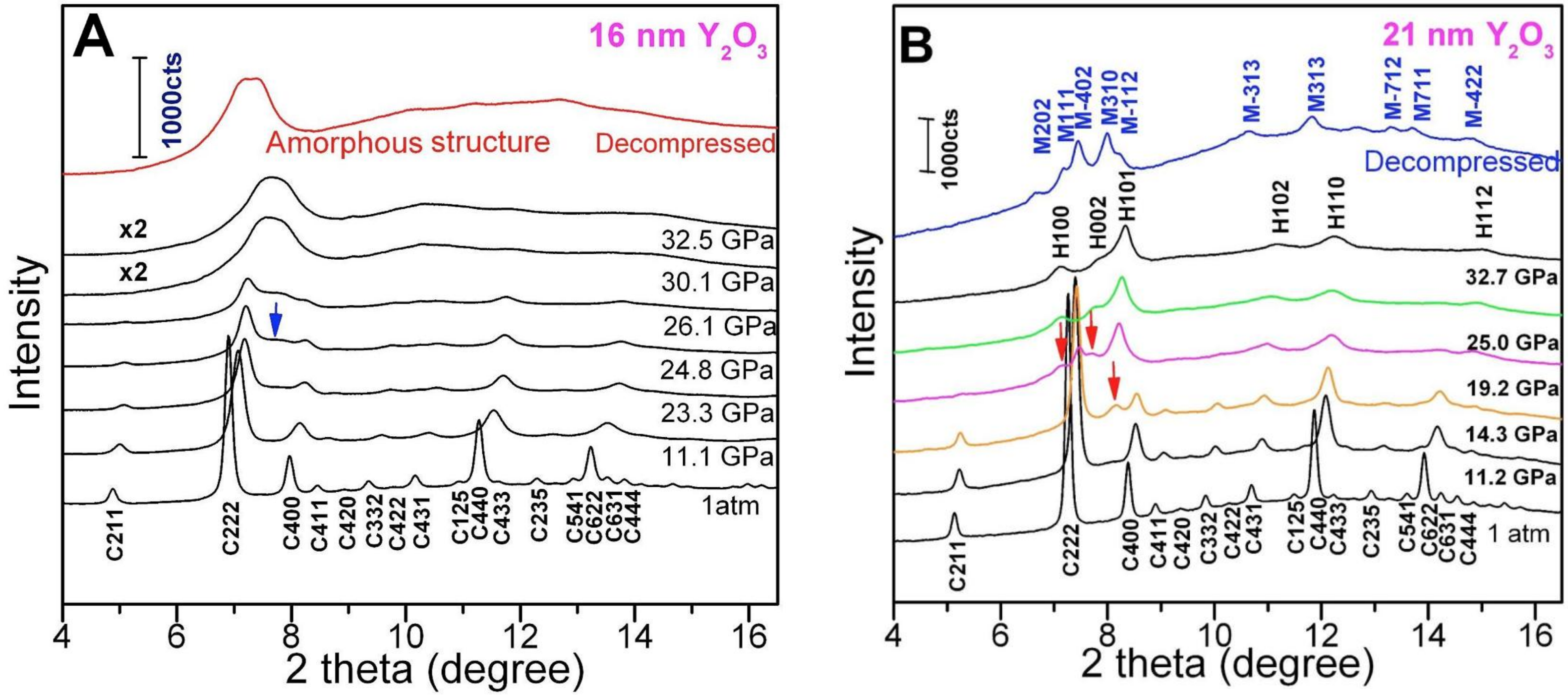


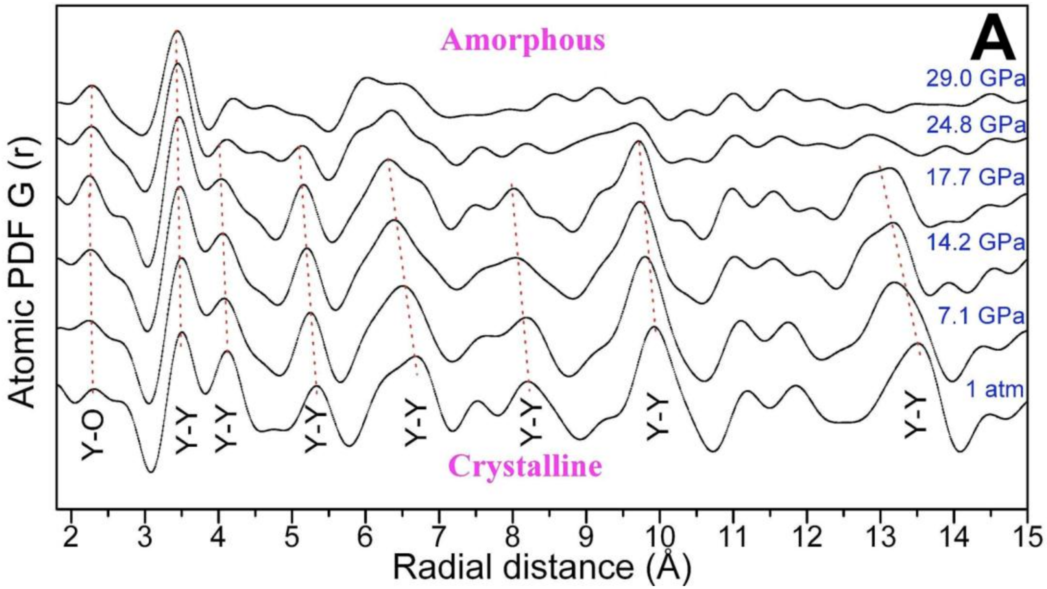
EFree Size-Dependent High-P Amorphization of Nanoscale Y_2O_3

Lin Wang, Wenge Yang, Yang Ding, Yang Ren,[4] Siguo Xiao, Bingbing Liu, Stanislav V. Sinogeikin, Yue Meng, David J. Gosztola, Guoyin Shen, Russell J. Hemley, Wendy L. Mao, & Ho-Kwang Mao,
PRL105, 095701 (2010)

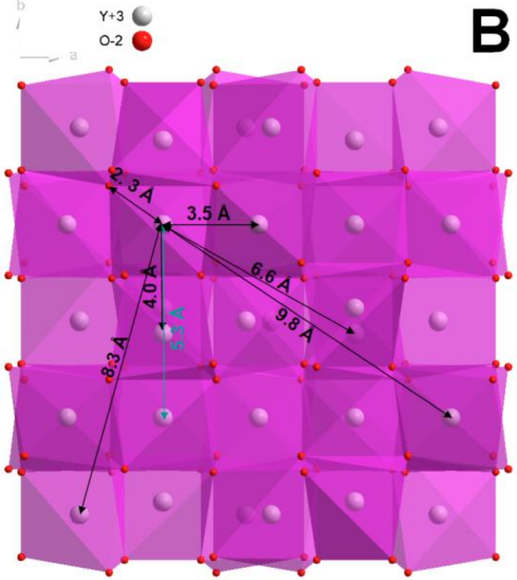


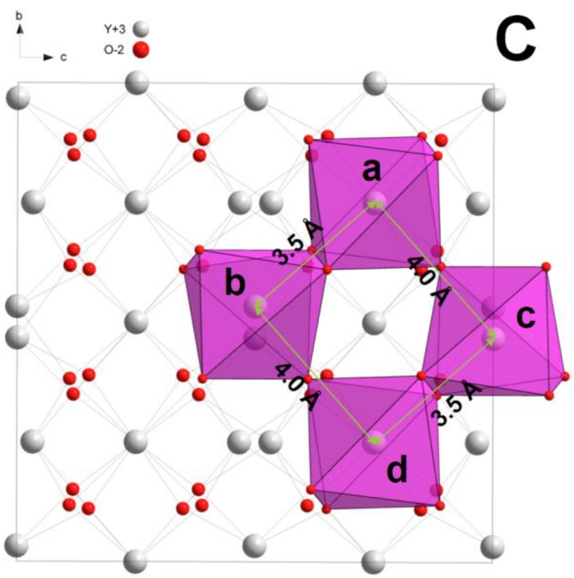
- Surface energy stabilizes the cubic Y_2O_3 and hindered its transition to monoclinic and hexagonal phases.
- Pressure breaks the linkages of YO_6 octahedra and amorphizes the crystal structure.
- The amorphous phase is recoverable after decompression

Size-Dependent High-P Amorphization of Nanoscale Y_2O_3



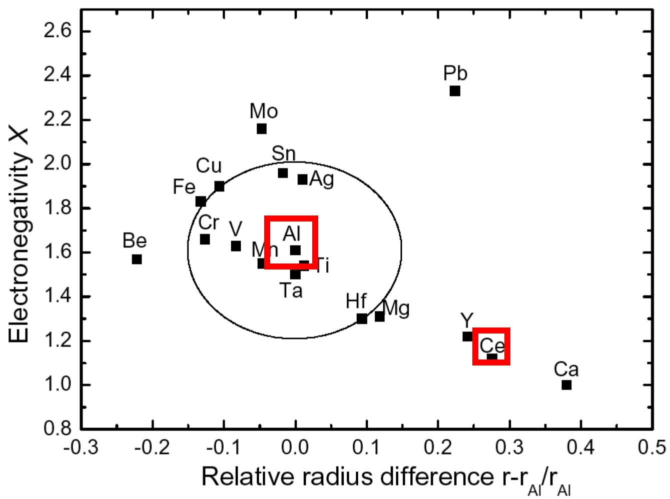
Lin Wang, *et al*, *Phys Rev Lett 105* 095701 (2010)

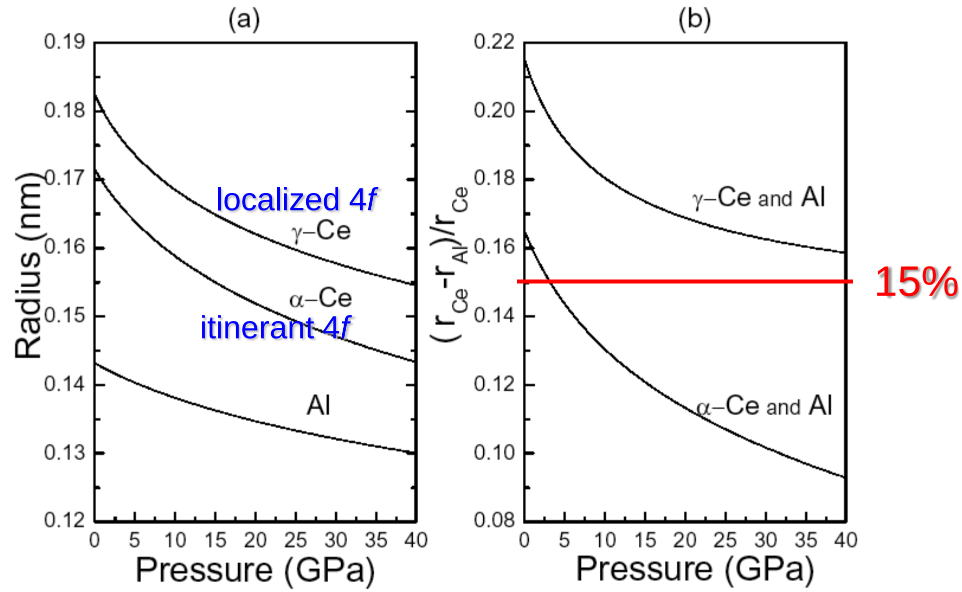




EFree

The formation of an unlikely alloy -- Ce_3Al



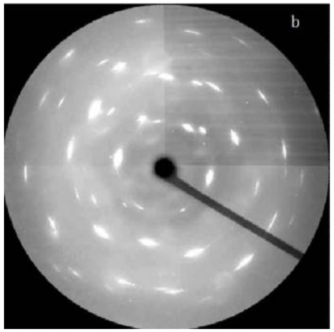


Hume-Ruthery Rule requires alloy components having similar atomic size & electronegativity.

Ce and Al are far apart and do not form alloy.

Pressure induces 4*f* delocallization in Ce, bringing atomic size and electronegativity of Ce close to Al.

Intermetallic compound and metallic glass Ce_3Al both convert to fcc alloy at high *P*. The novel alloy is stable when quenched to 1 bar.



XRD pattern of quenched fcc Ce3Al alloy

Zeng *et al*, *PNAS* (2009), Zeng *et al.*, *Phys. Rev. Lett.* (2010)

PRL **104,** 105702 (2010) PHYSICAL REVIEW LETTERS week ending 12 MARCH 2010

Origin of Pressure-Induced Polyamorphism in $Ce_{75}Al_{25}$ Metallic Glass

Qiao-shi Zeng,[1,2] Yang Ding,[2] Wendy L. Mao,[1,3,4,5] Wenge Yang,[2,6] Stas. V. Sinogeikin,[6] Jinfu Shu,[7] Ho-kwang Mao,[1,2,6,7] and J. Z. Jiang[1,*]

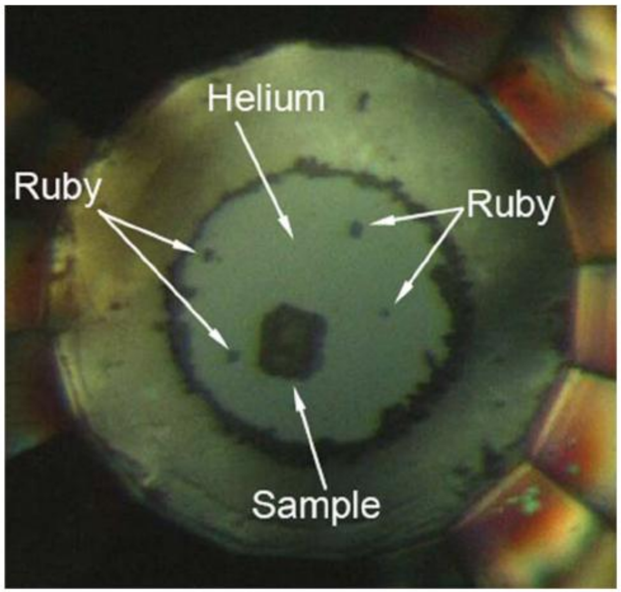
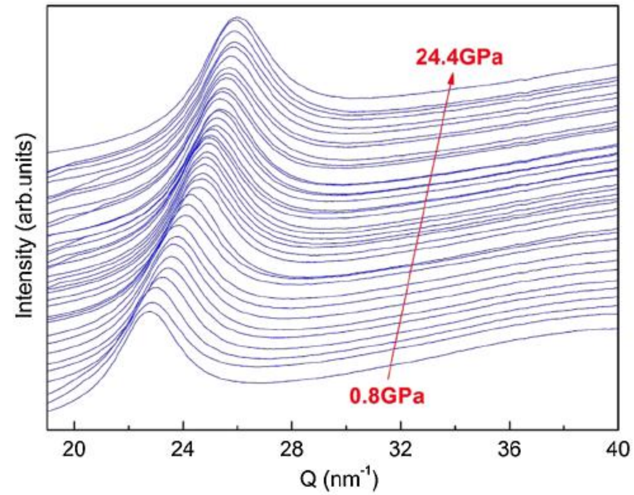
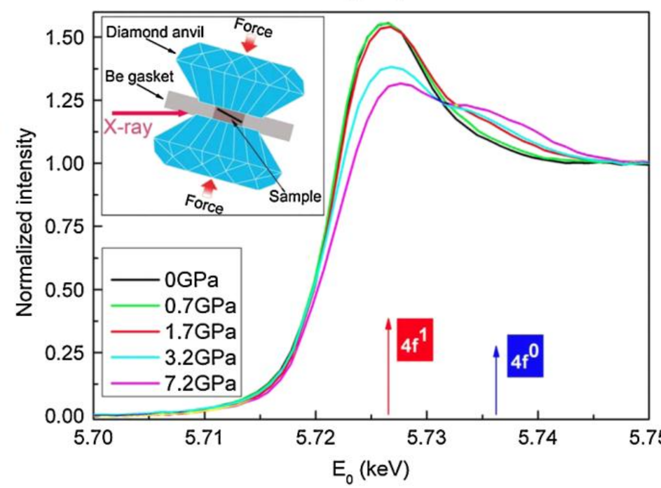


FIG. 1 (color online). Photomicrograph of sample loaded with helium in DAC at 0.8 GPa.



XRD



Ce L_3-edge XANES

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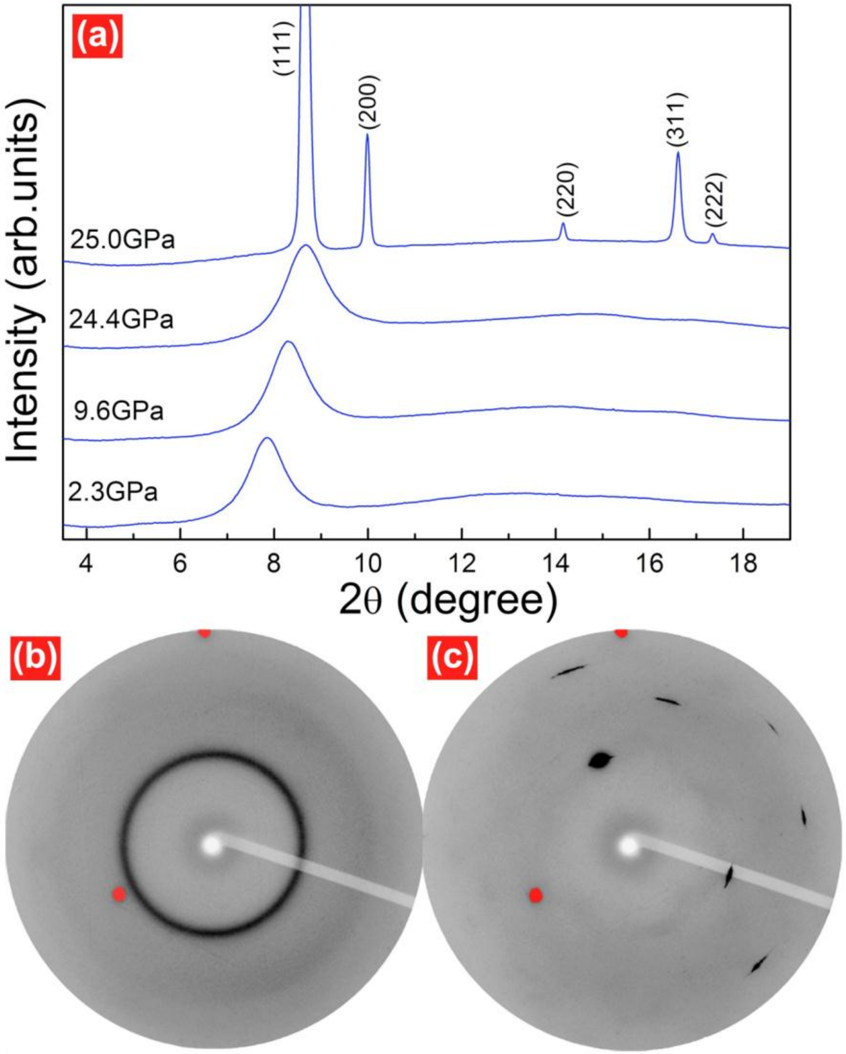
Glass with Long-Range Topological Order



- Challenging the fundamental concept, "glass does not have long-range order."
- $Ce_{75}Al_{25}$ metallic glass crystallizes into a large single crystal at high pressure
- indicating a long-range topological order.

- metallic glass at the cutting-edge materials research
- Combination of high-*P* synchrotron x-ray diffraction, x-ray spectroscopy, electron diffraction, high-resolution TEM, and molecular dynamic simulation
- The discovery at high P is recoverable

Qiaoshi Zeng, Hongwei Sheng, Yang Ding, Lin Wang, Wenge Yang, Jian-Zhong Jiang, Wendy L. Mao, and Ho-Kwang Mao, *Science 332,* 1404 (2011)

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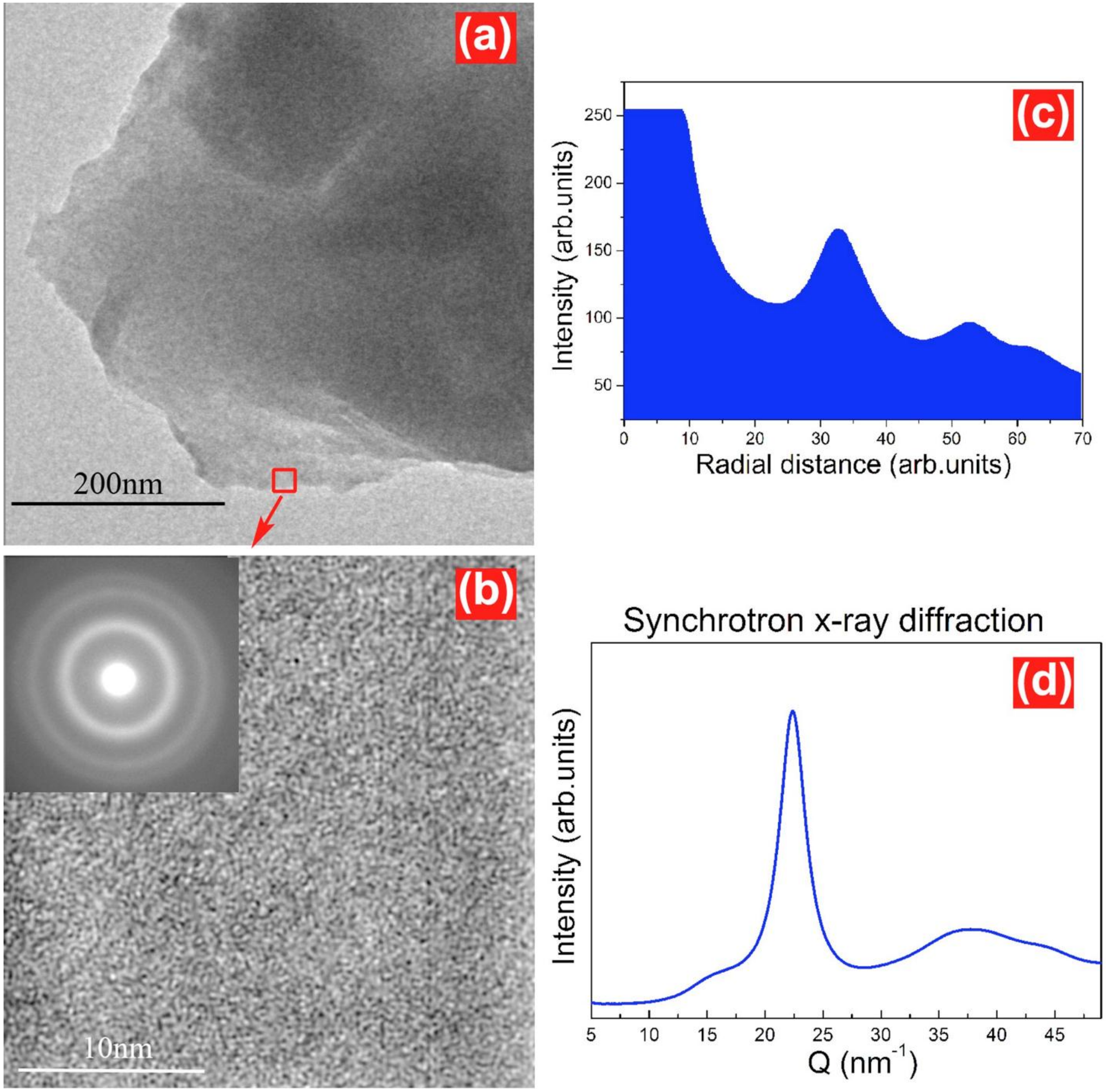
$Ce_{75}Al_{25}$ metallic glass

The sample: HRTEM image electron diffraction and x-ray diffraction show a typical amorphous glass patterns

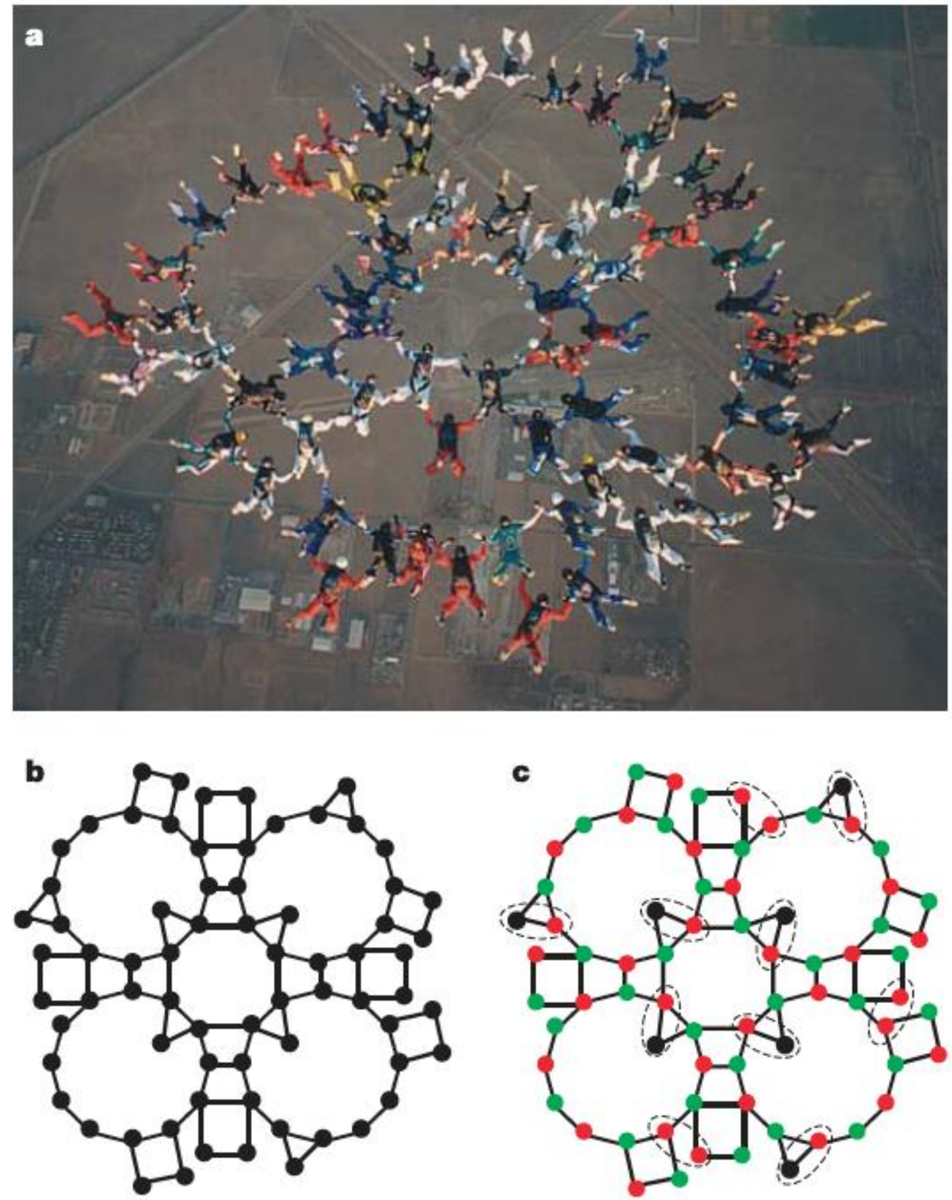


What is long-range topological order?

Topological versus chemical ordering in network glasses at intermediate and extended length scales

Philip S. Salmon[1], Richard A. Martin[1], Philip E. Mason[1] & Gabriel J. Cuello[3]

NATURE | VOL 435 | 5 MAY 2005 |



- Only medium-range topological order has been observed in glass.
- Long-range topological order would mean a “perfect glass” according to the Kauzmann paradox.

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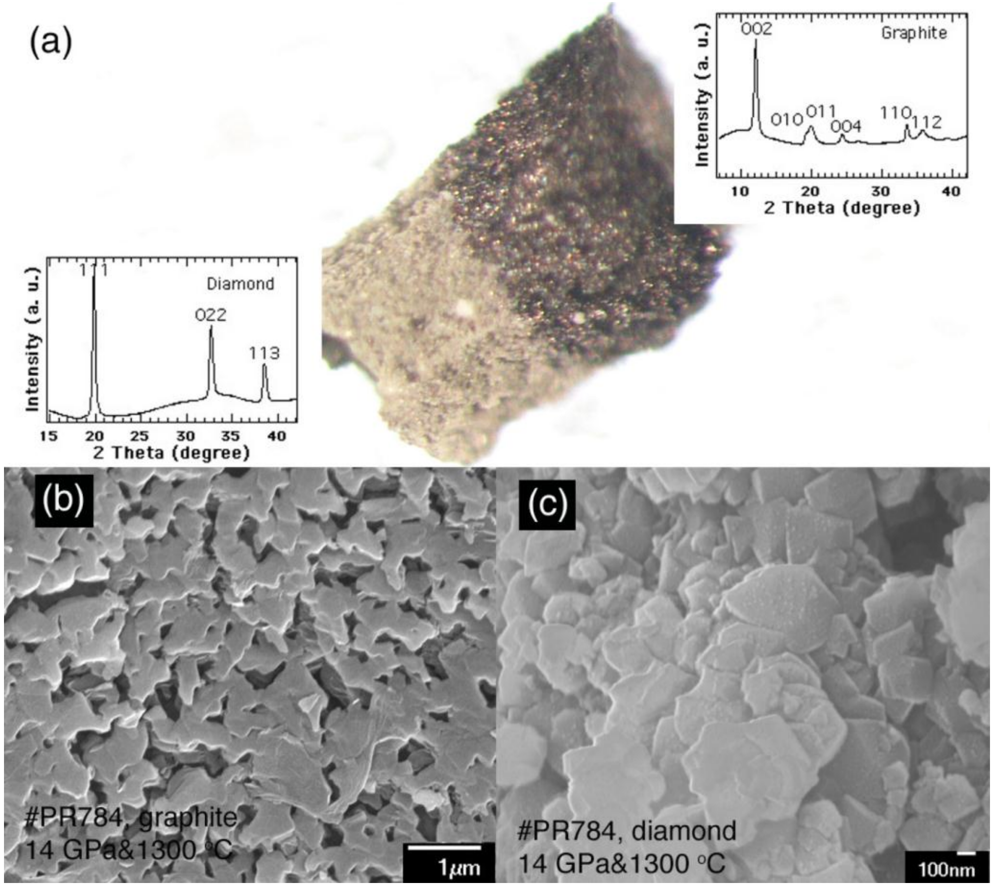
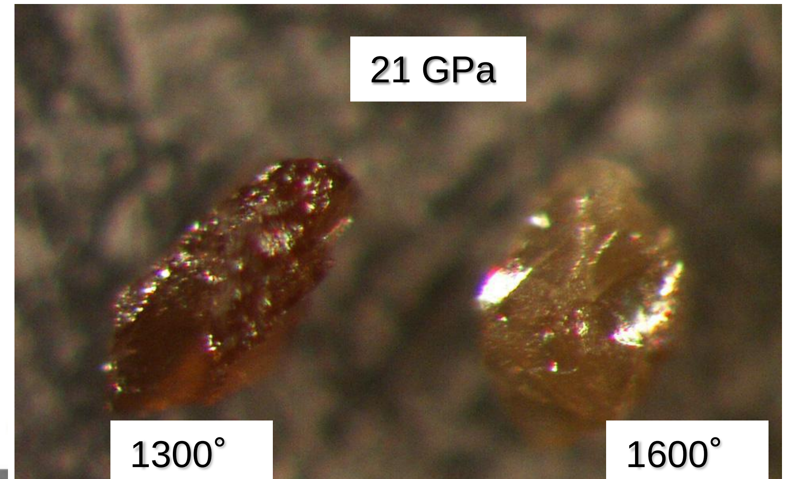
Conversion of mesoporous carbon to mesoporous diamond





- Pores in mpC survive 21 GPa!
- mp-diamond as a superhard novel material
- Combination of high-*P* MAS, x-ray diffraction, Raman spectroscopy, & electron microscopy
- The high-*P* product is recoverable

Li Zhang, Paritosh Mohanty, Neil Coombs, Yingwei Fei , Ho-Kwang Mao, Kai Landskron, *Proc. Nat. Acad. Sci. USA 107,* 13893-13896 (2010)

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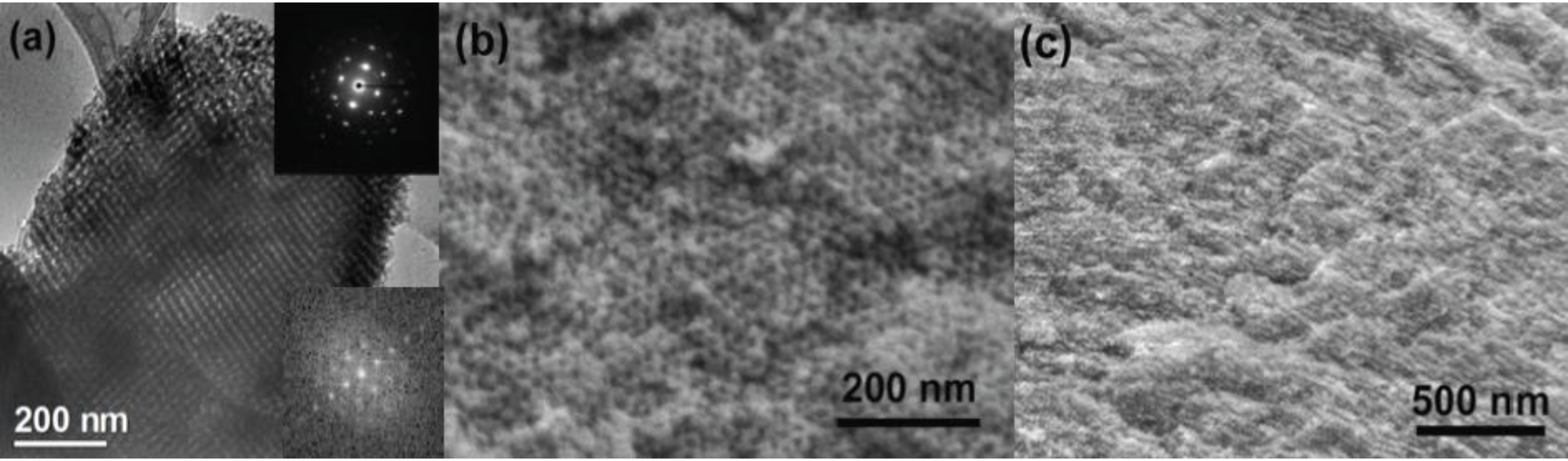
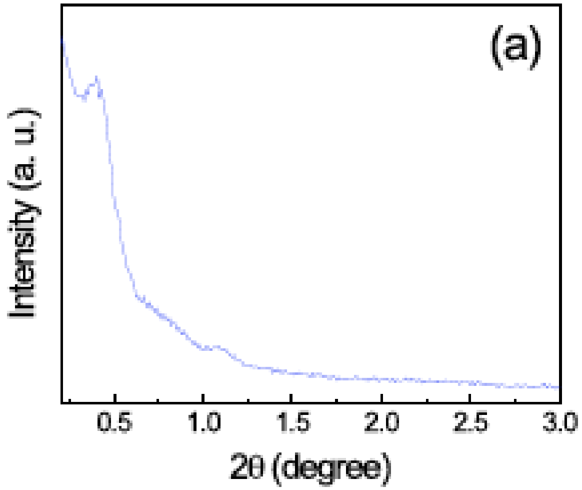
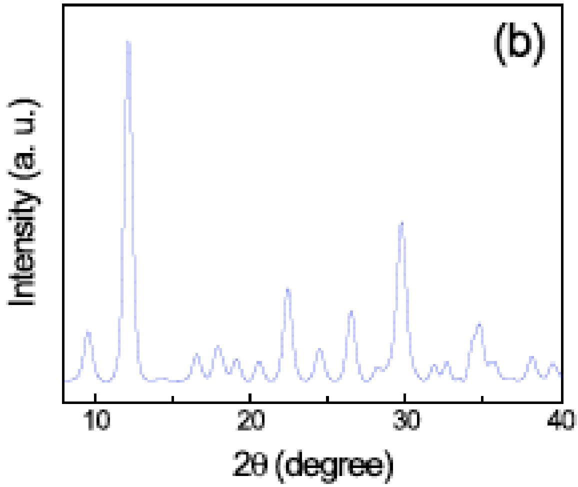
HP conversion of mp-silica to mp-quartz

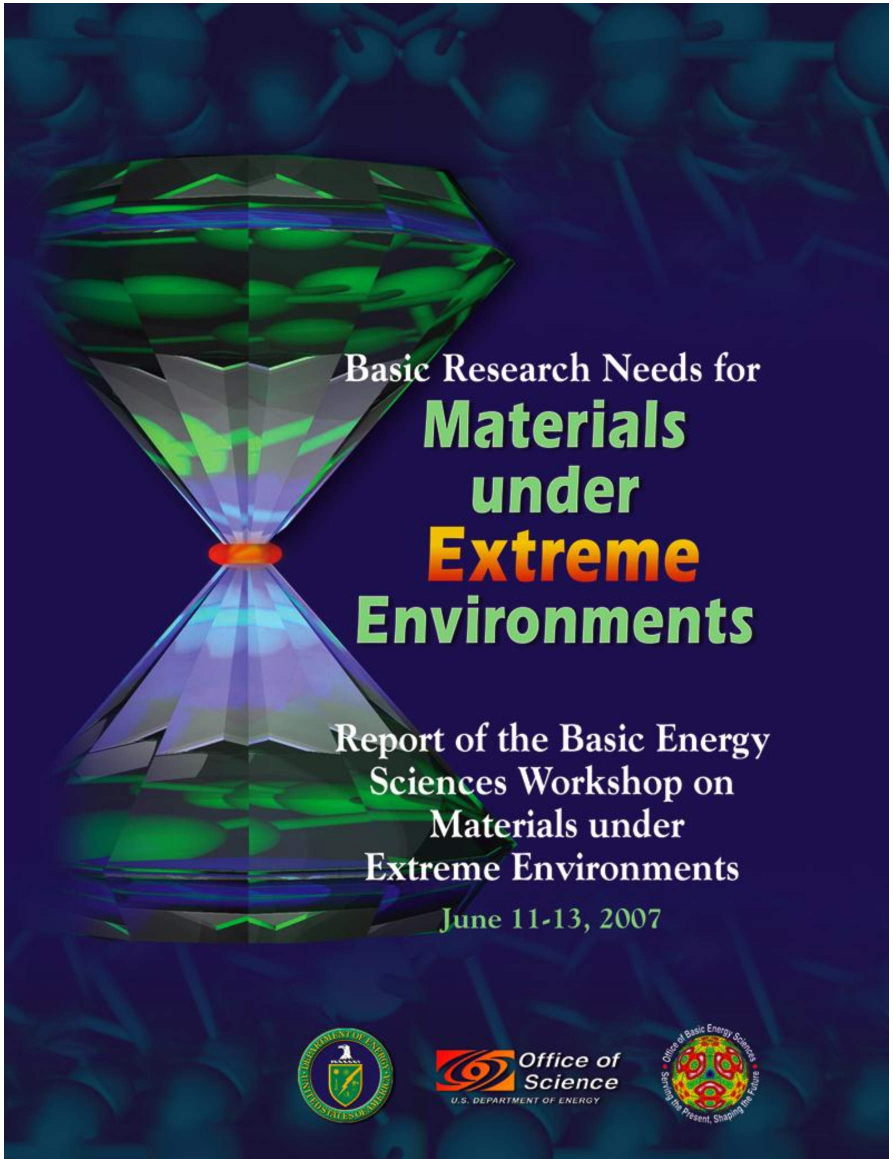
Paritosh Mohanty, Manuel Winberger, Yingwei Fei, Kai Landskron, *JACS in press* (2011)







- Conversion at 4 GPa 550° C
- Periodic fcc pores
- 15 nm connected pores
- Quartz is inert in hydrothermal environment
- Potential as molecular sieve



EFree advantages

- The vast field of materials with extremely favorable properties
- Unprecedented alliance of the best minds
- Unprecedented assemblage of powerful enabling tools
- **Discovery at high *P***
- **Recovery for applications**
- **Materials by design**
- **Focusing on Energy**