Solids under extreme pressure

Dr Taras Palasyuk

Institute of Physical Chemistry PAS

„This is but the least
we have yet seen of the work of the Lord,
much is still hidden from us”

Carl Linnaeus

03.11.2016
PhD Symposium, Institute of Physics PAS

OUTLINE

- **Brief introduction on the neccessity of high-pressure research**
- **Basics of diamond anvil cell technique**
- **Examples of modern cutting edge investigations of matter under extreme conditions:**

„Looking" throughout Sodium
on inducing an insulating state in elemental sodium

Squeezing „salt" out of Ammonia
on the proton transfer between neutral amonia molecules

Irresistable „smell" of Hydrogen
on high- temperature superconductivity in hydrogen dominant materials

„Turning" Nitrogen into diamond
on transformation of molecular nitrogen to single-bonded atomic solid

New „taste" of chemistry
on unexpected chemical composition

„Ground"-breaking news
on possible processes at high-pressure high-temperature conditions
similar to the Earth's interior

Why is research at high pressure important ?

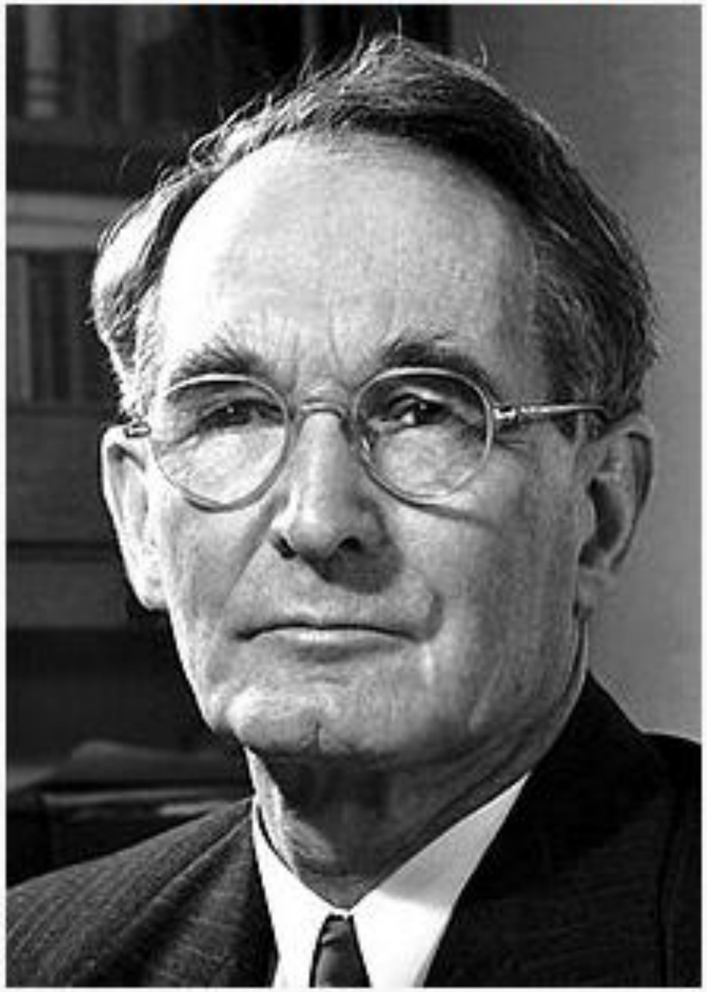
What pressure range would be of interest for study ?

How can pressure be generated ?

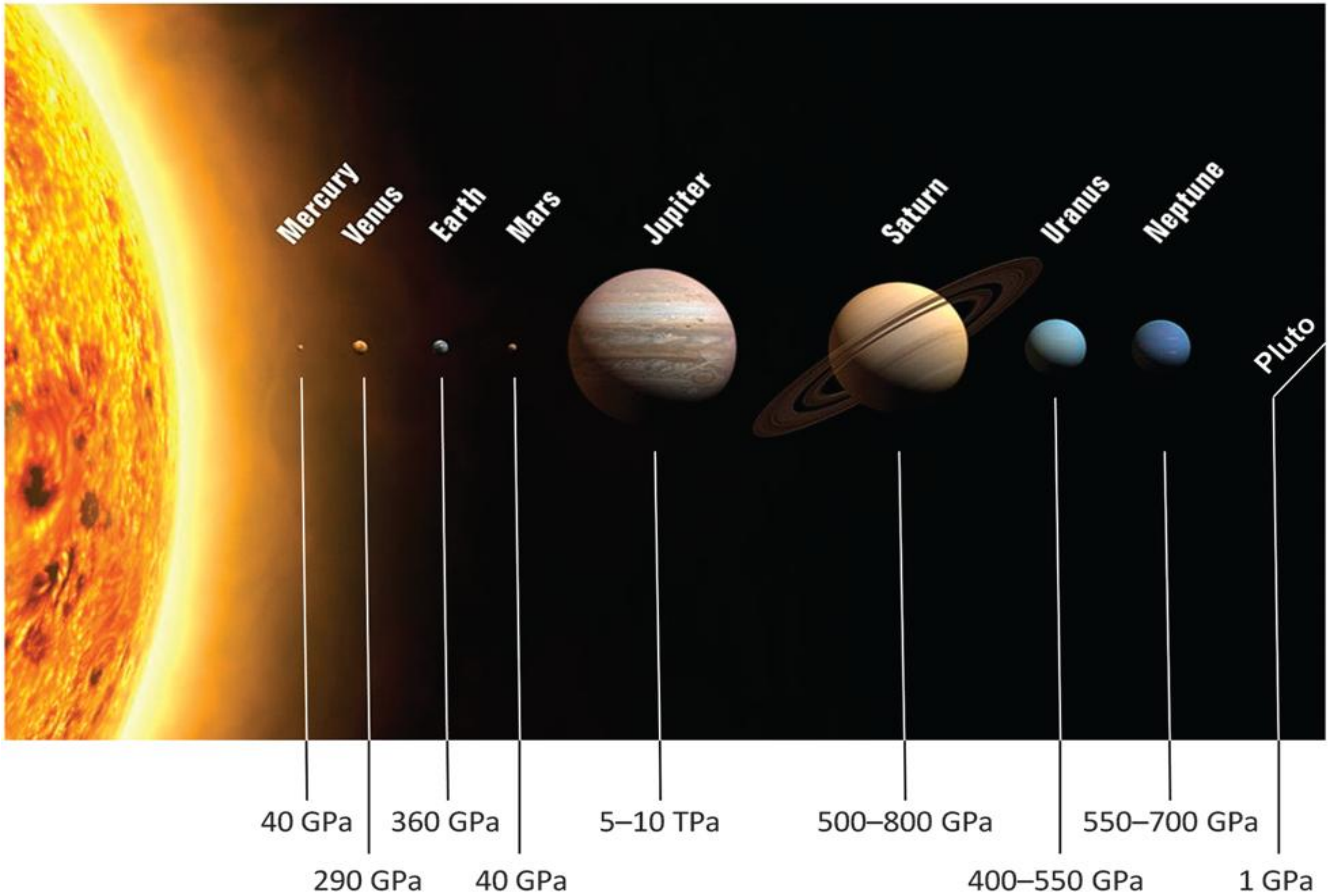
1946 - Nobel prize in Physics

Pressure range up to 10 GPa (10 000 atm)

Percy Williams Bridgman



Pressure in the Universe: 10^{-32} do 10^{32} atm.



1 GPa = 10^3 atm

Pressure in Laboratory: od ~10^{-20} do ~$5x10^6$ atm.

E. Zurek and W. Grochala
Predicting crystal structures and properties of matter under extreme conditions *via* quantum mechanics: the pressure is on
PhysChemChemPhys 17 (2015) 2917

Generation of pressure

static techniques

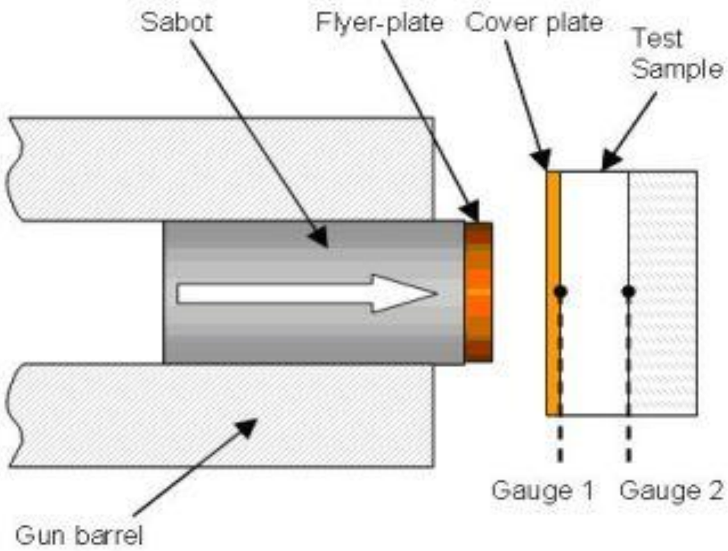
Piston-cylinder
(~2 GPa)

Multi-anvil technique
(~50 GPa)

Anvil Cell
(~ 500 GPa)

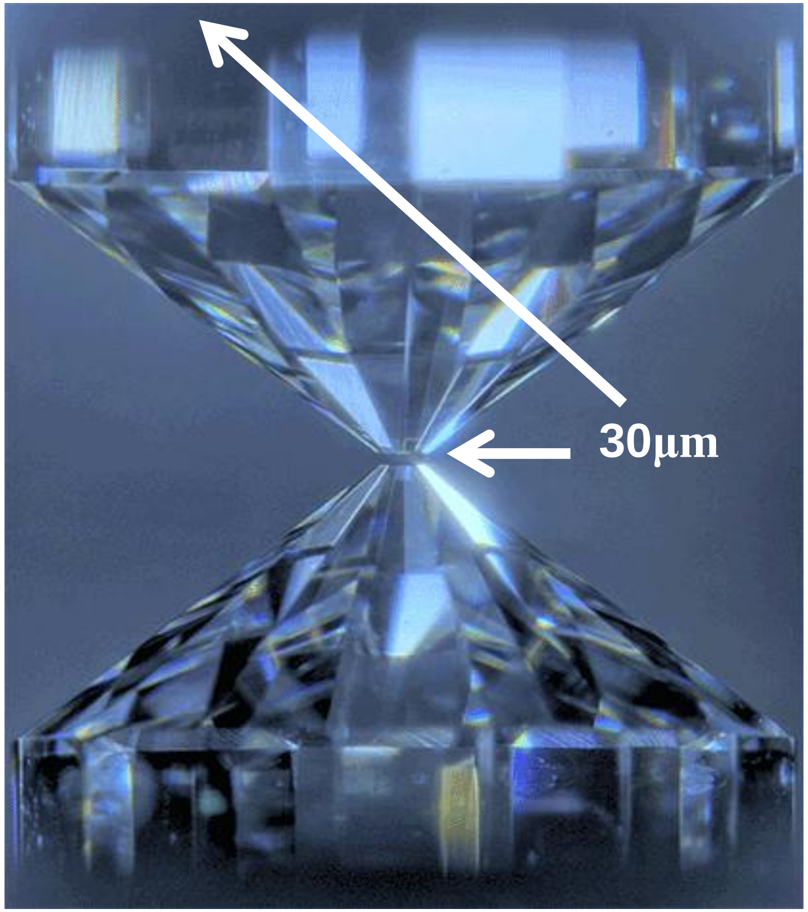
dynamic techniques

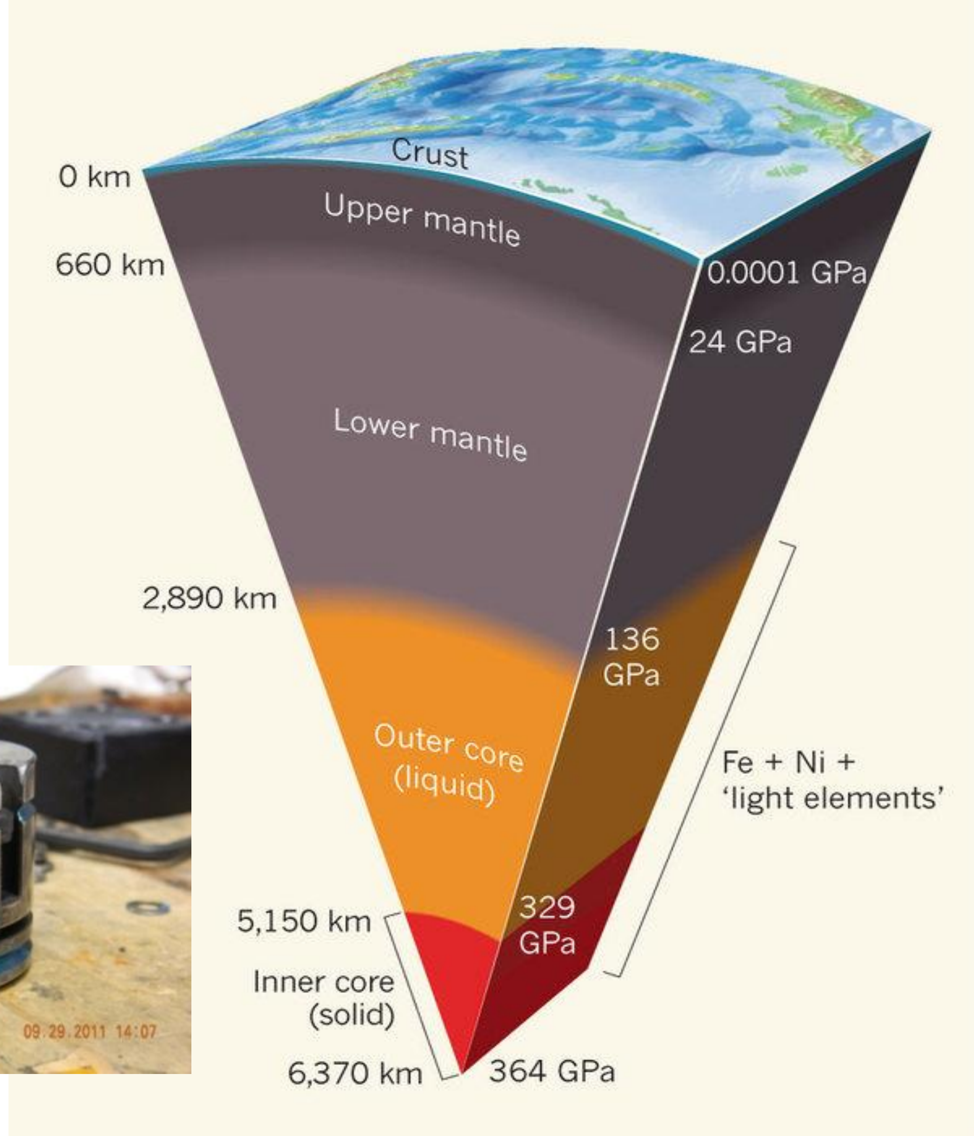
-Shock wave technique
(~ 300 GPa)



simple tool → astonishing effect

record pressure attained with DAC
~ 5 Mbar (5x10⁶ atm)





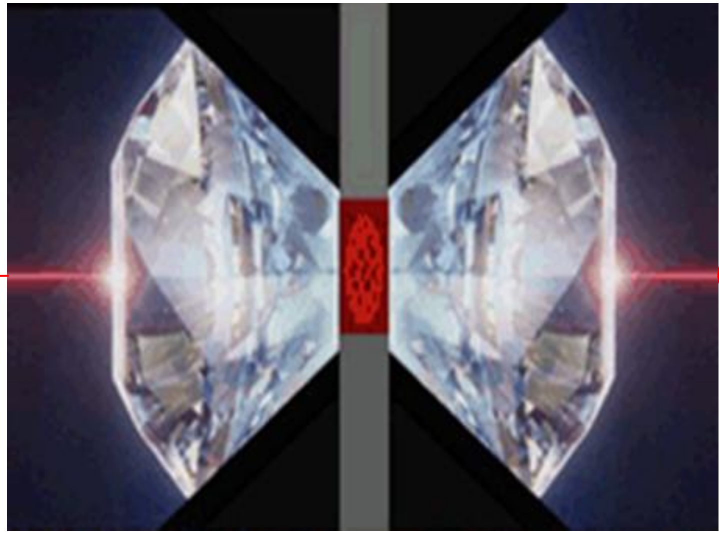
Diamond Anvil Cell - DAC

Diamond Anvils are suitable for various analytical techniques

X–ray,
neutron

Laser (UV, Vis, IR)

γ-ray



X-ray/neutron diffraction

X-ray absorption study

Raman spectroscopy

IR absorption

Nuclear Resonant Scattering

Mößbauer spectroscopy

Brillouin scattering

„Looking” throughout Sodium

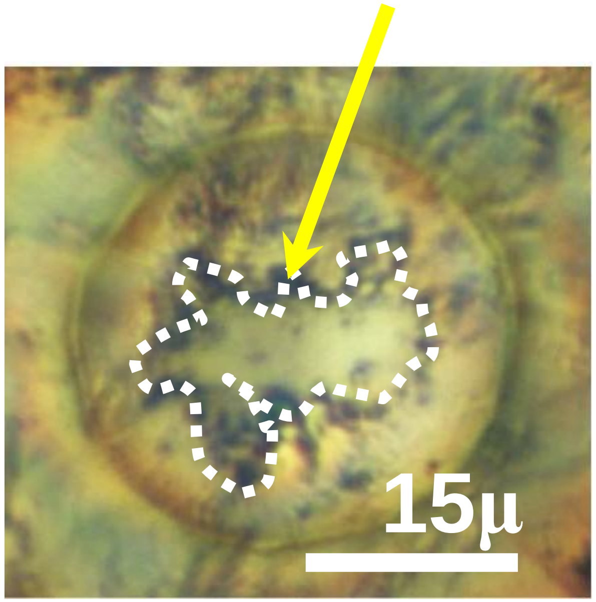
nature
12 MARCH 2009

Transparent dense sodium

Yanming Ma[1,2], Mikhail Eremets[3], Artem R. Oganov[2,4]†, Yu Xie[1], Ivan Trojan[3], Sergey Medvedev[3], Andriy O. Lyakhov[2]†, Mario Valle[5] & Vitali Prakapenka[6]

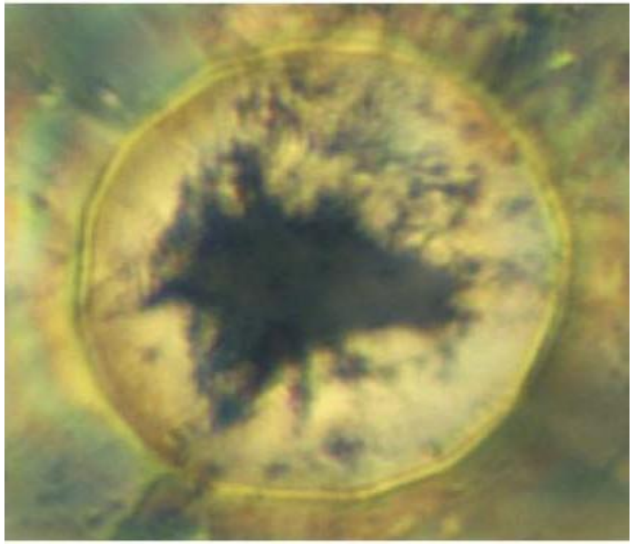
EXPERIMENT

sample



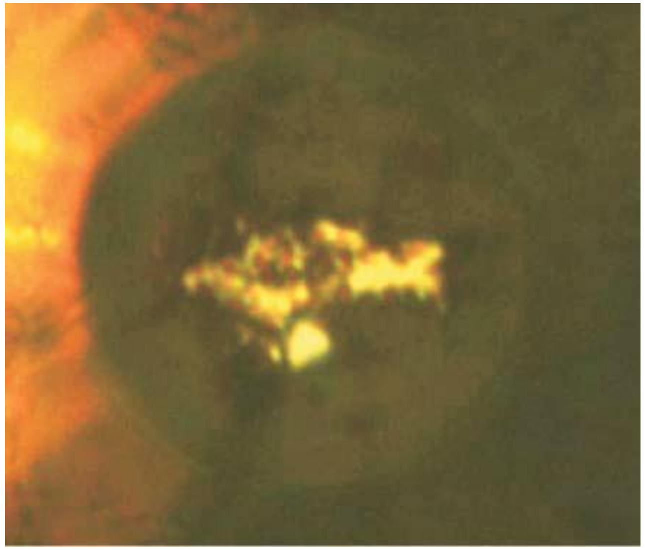
120 GPa

Reflected light



156 GPa

Reflected light



199 GPa

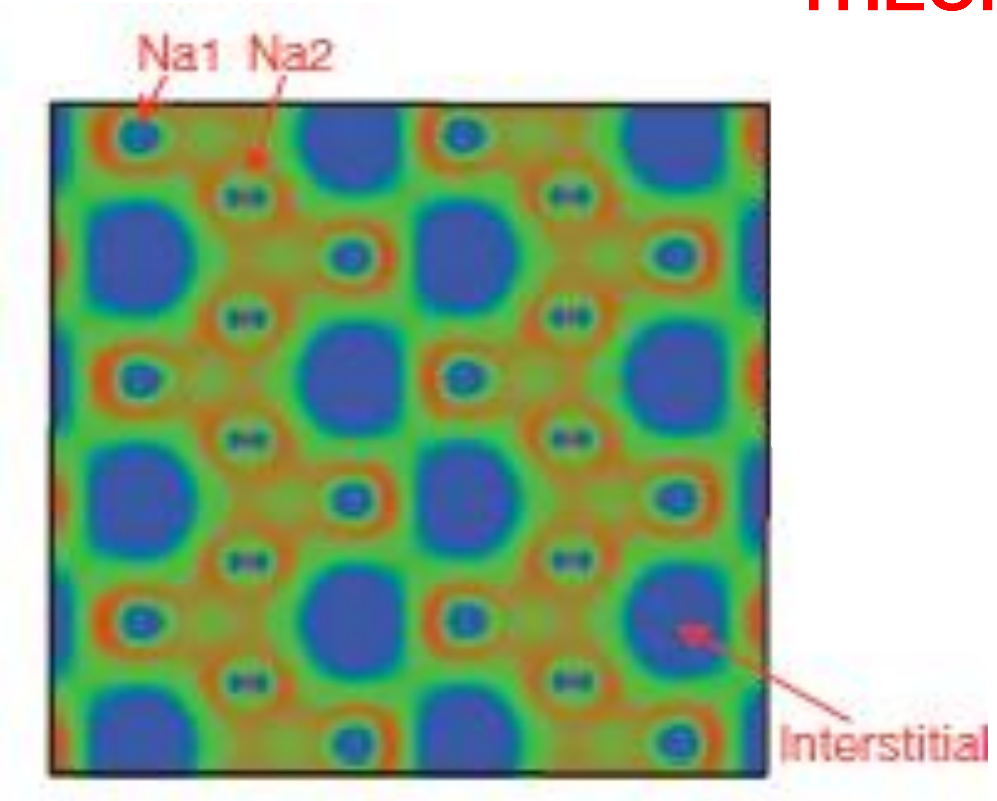
Transmitted light

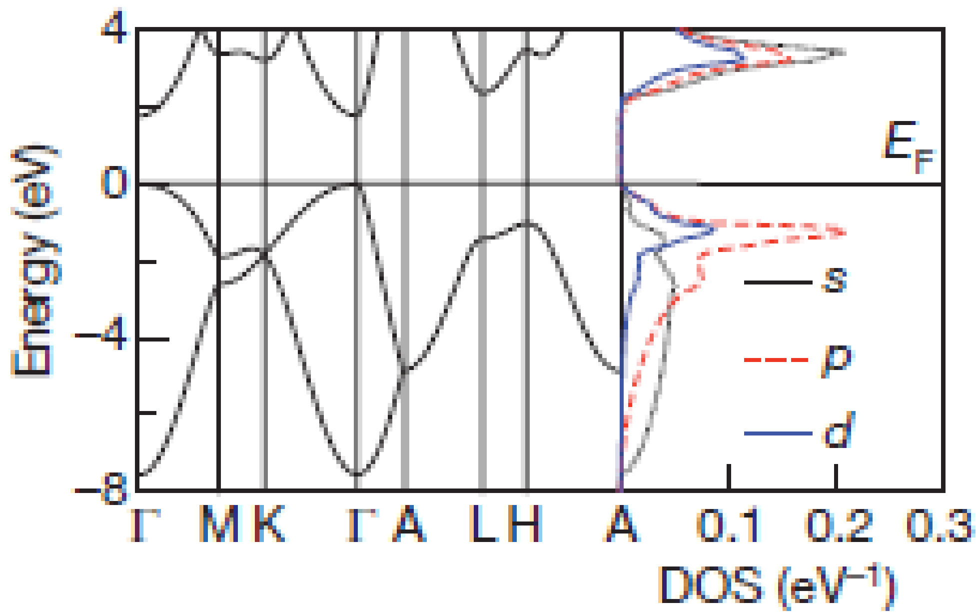
nature
12 MARCH 2009

Transparent dense sodium

Yanming Ma[1,2], Mikhail Eremets[3], Artem R. Oganov[2,4]†, Yu Xie[1], Ivan Trojan[3], Sergey Medvedev[3], Andriy O. Lyakhov[2]†, Mario Valle[5] & Vitali Prakapenka[6]

THEORY



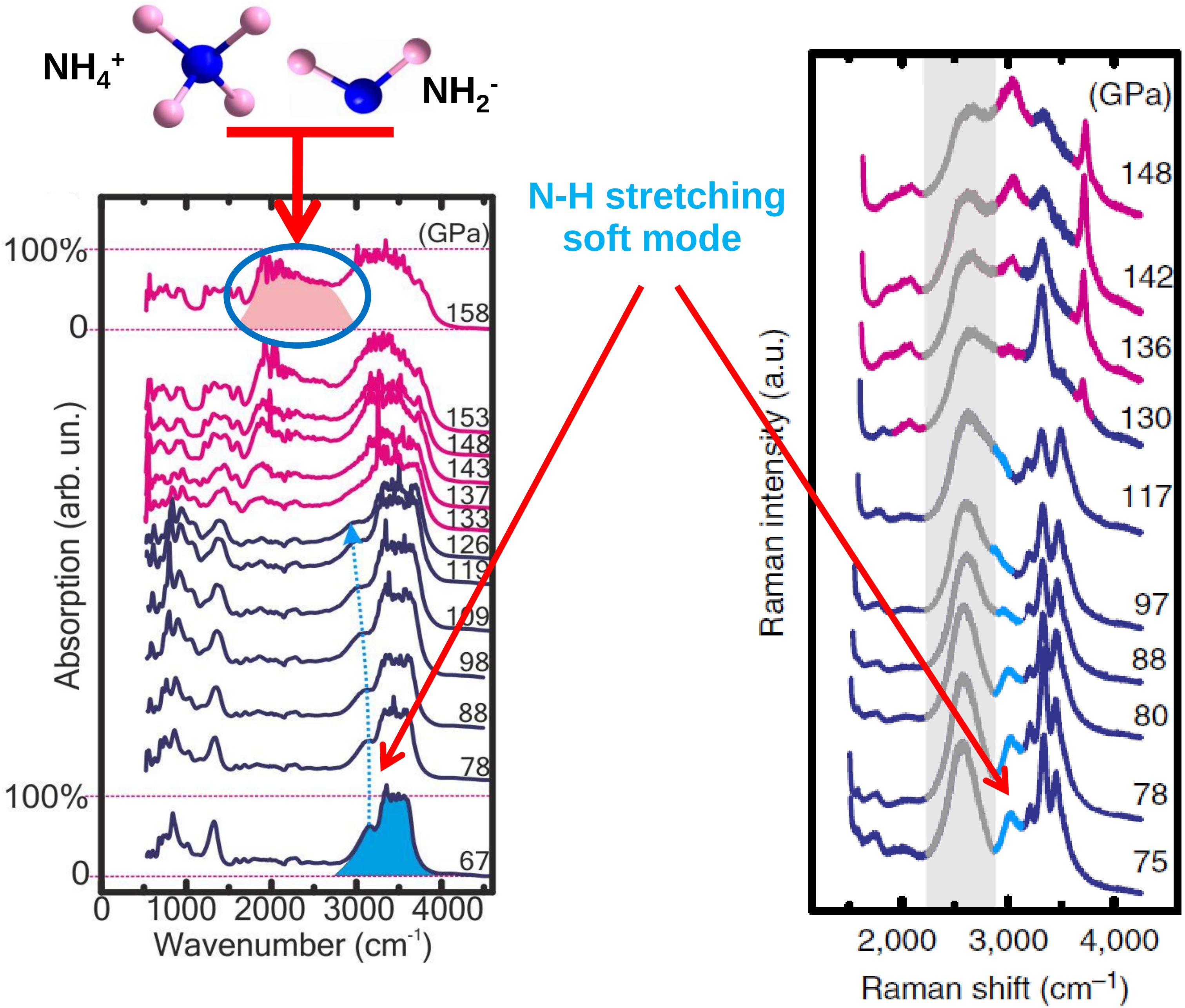


Overlapping sodium atoms force their outer electrons into the "holes" between the atoms.
Increased hybrydization of 3*d* and 3*p* bands induces strong localization of electrons and subsequent gap opening.

Squeezing „salt” out of Ammonia

nature COMMUNICATIONS
Received 19 Oct 2013 | Accepted 17 Feb 2014 | Published 24 Mar 2014
DOI: 10.1038/ncomms4460

Ammonia as a case study for the spontaneous ionization of a simple hydrogen-bonded compound



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Ammonia as a case study for the spontaneous ionization of a simple hydrogen-bonded compound

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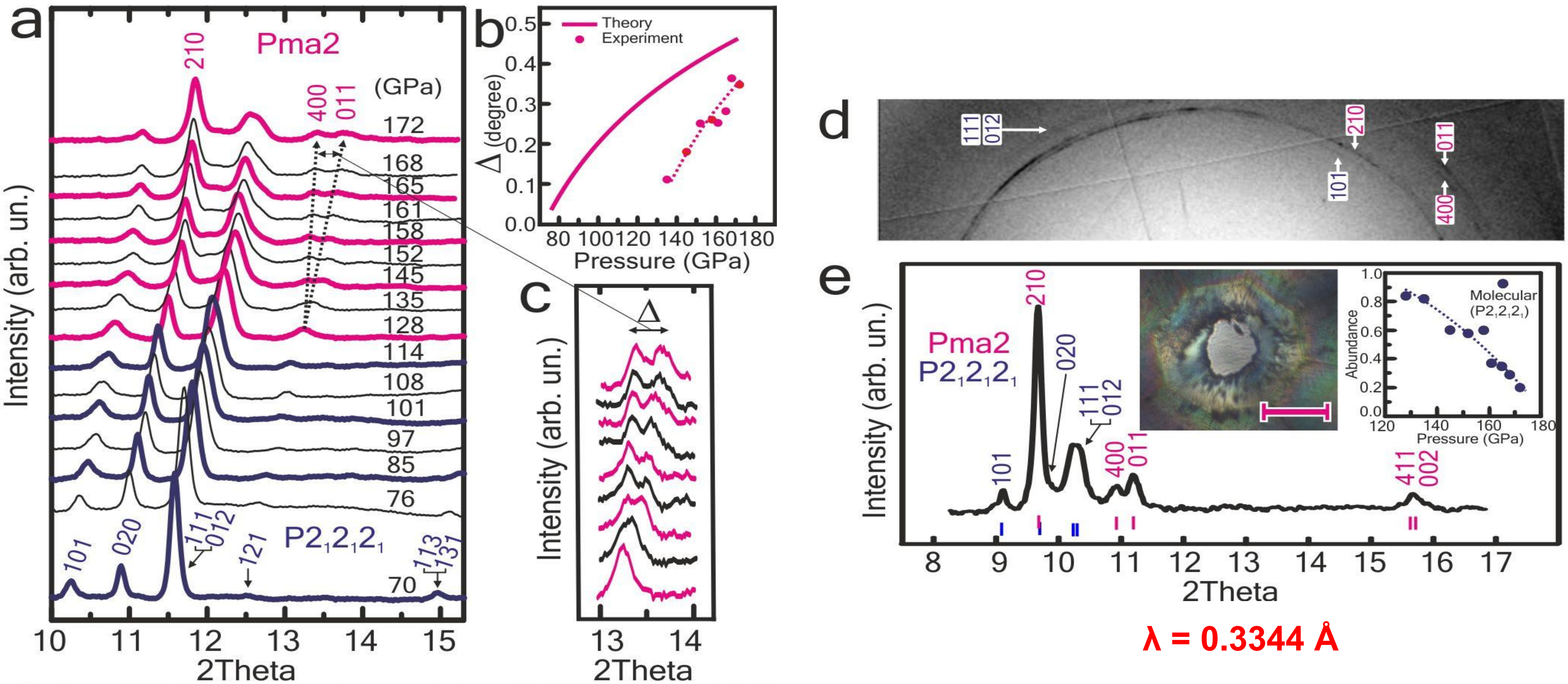

λ = 0.4125 Å

λ = 0.3344 Å

nature COMMUNICATIONS
Received 19 Oct 2013 | Accepted 17 Feb 2014 | Published 24 Mar 2014
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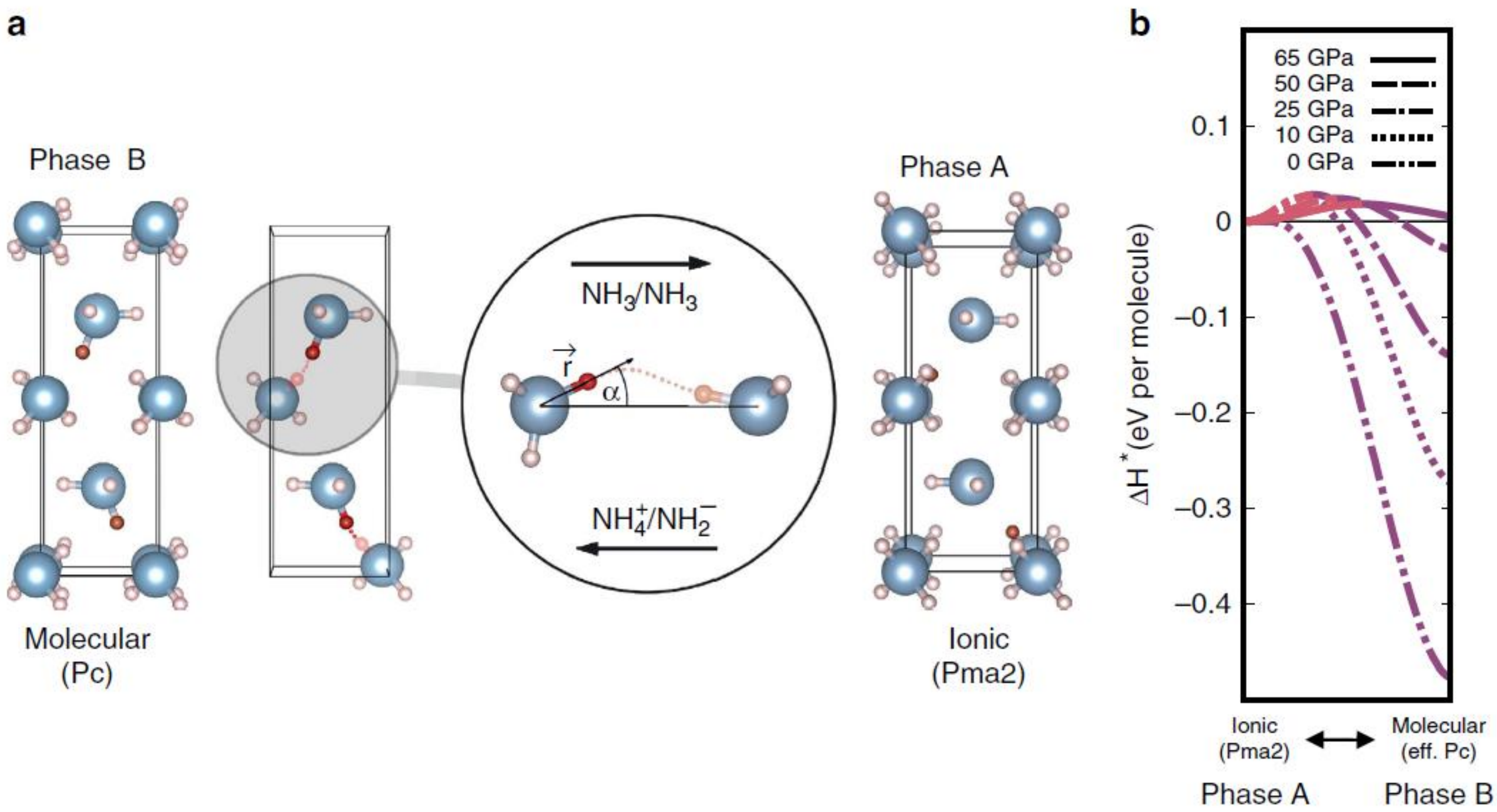


Irresistable „smell” of Hydrogen

VOLUME 92, NUMBER 18 PHYSICAL REVIEW LETTERS week ending 7 MAY 2004

Hydrogen Dominant Metallic Alloys: High Temperature Superconductors?

N.W. Ashcroft

Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853-2501, USA
Donostia International Physics Center, San Sebastian, Spain

(Received 29 December 2003; published 6 May 2004)

The arguments suggesting that metallic hydrogen, either as a monatomic or paired metal, should be a candidate for high temperature superconductivity are shown to apply with comparable weight to alloys of metallic hydrogen where hydrogen is a dominant constituent, for example, in the dense group IVa hydrides. The attainment of metallic states should be well within current capabilities of diamond anvil cells, but at pressures considerably lower than may be necessary for hydrogen.

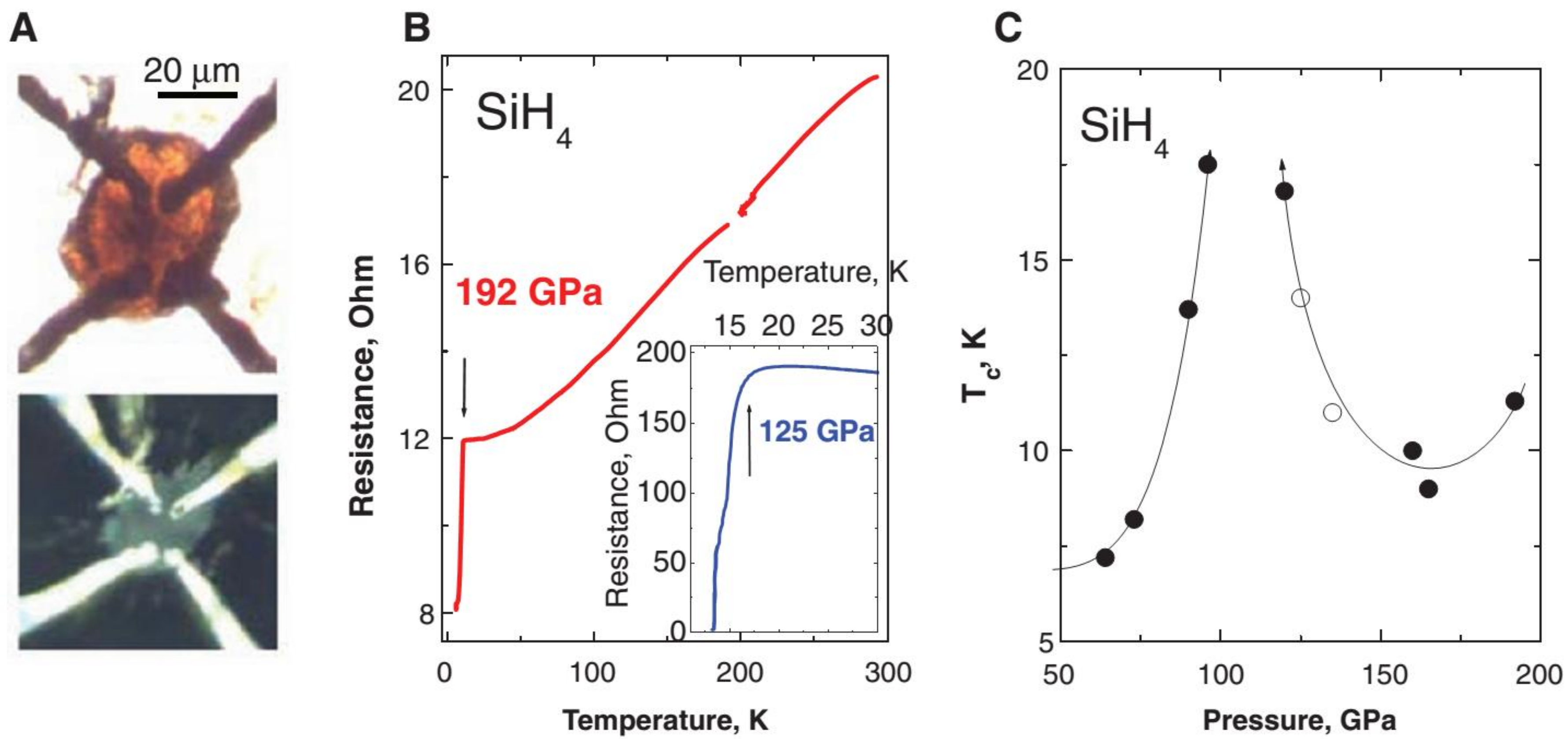
DOI: 10.1103/PhysRevLett.92.187002 PACS numbers: 74.10.+v, 71.30.+h

Science
AAAS

Superconductivity in Hydrogen Dominant Materials: Silane

M. I. Eremets[1,*], I. A. Troian[1,†], S. A. Medvedev[1], J. S. Tse[2], Y. Yao[2]

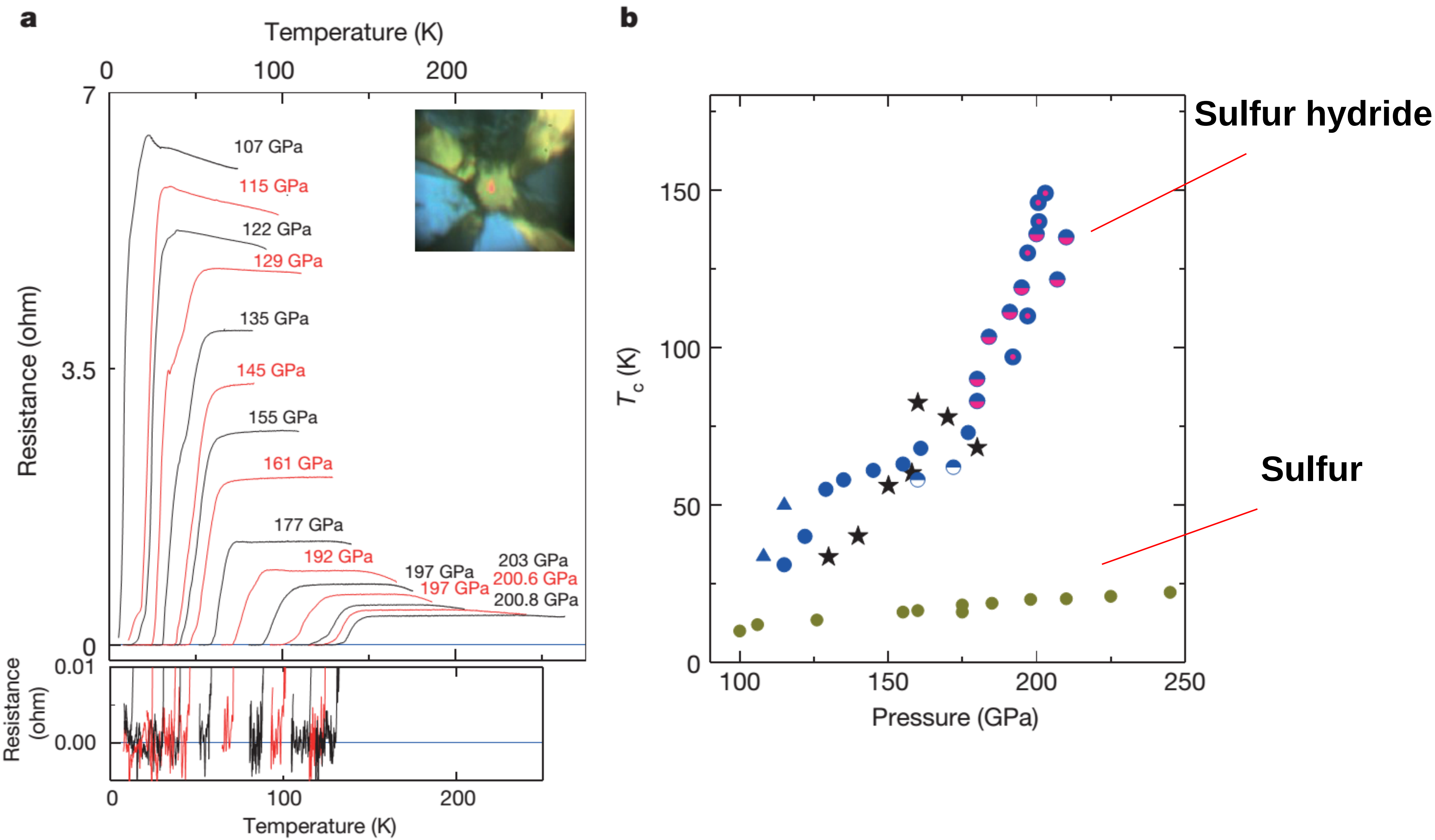
14 MARCH 2008



nature
17 AUGUST 2015

Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system

A. P. Drozdov[1]*, M. I. Eremets[1]*, I. A. Troyan[1], V. Ksenofontov[2] & S. I. Shylin[2]



nature
17 AUGUST 2015

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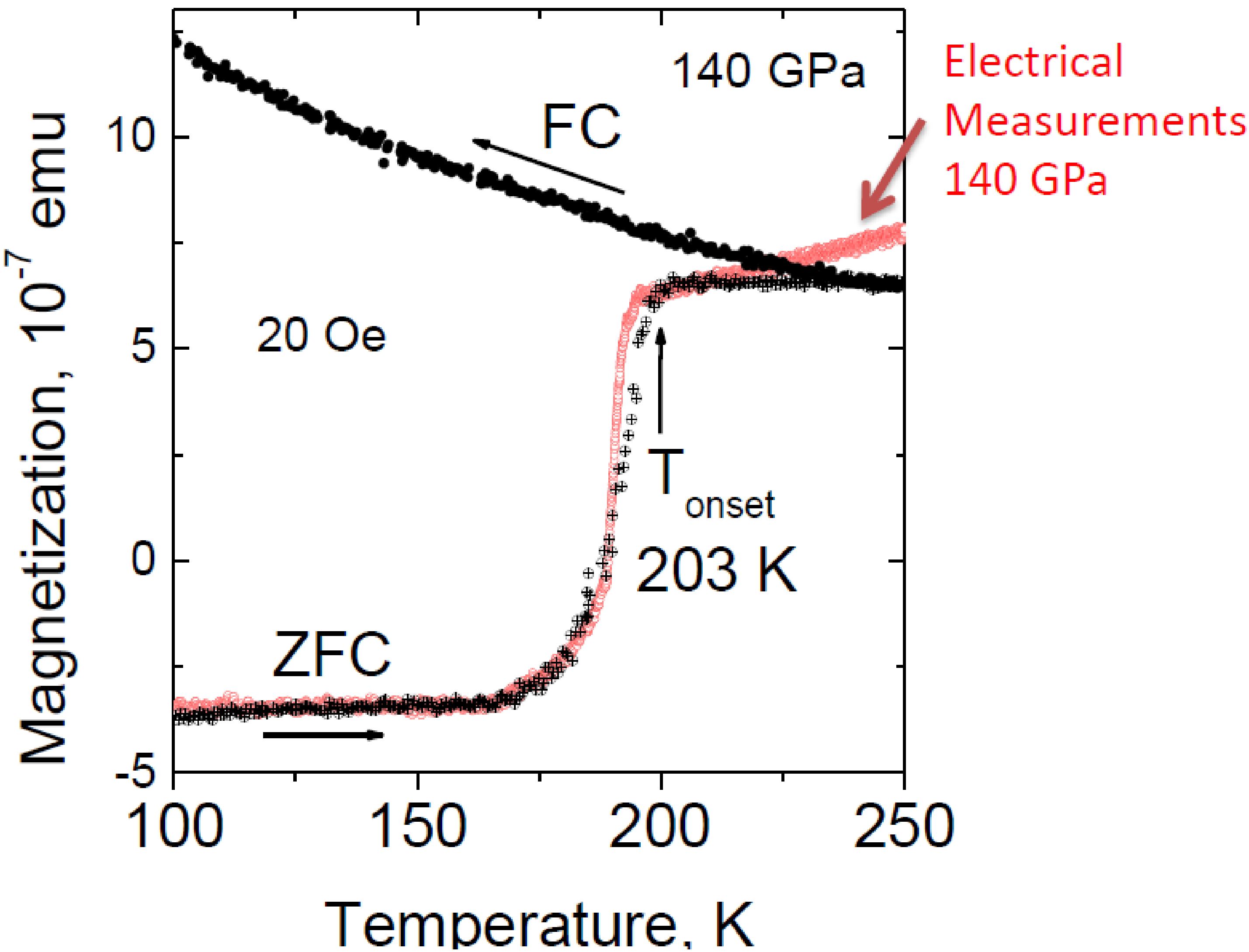
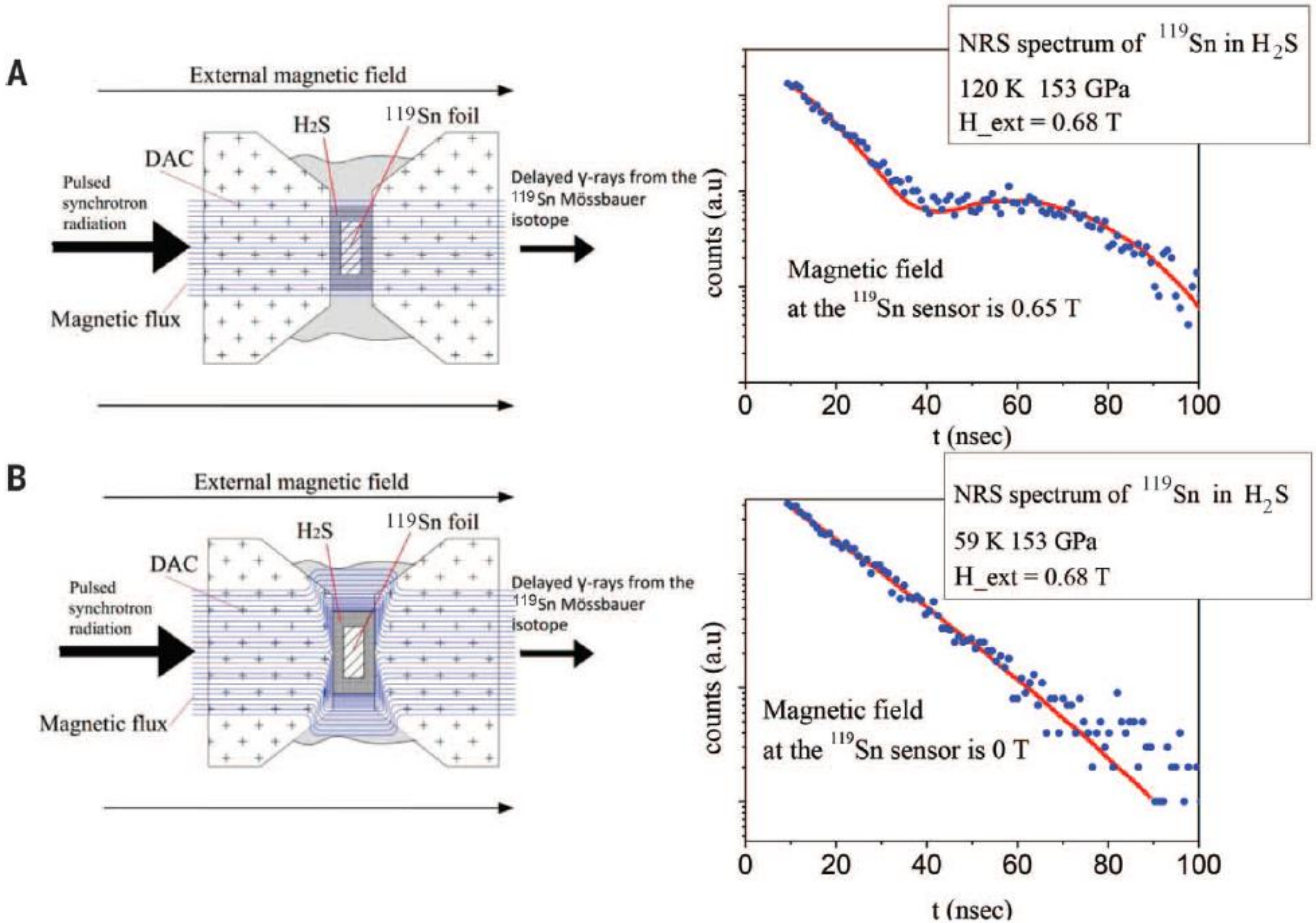


Science AAAS

18 MARCH 2016

Observation of superconductivity in hydrogen sulfide from nuclear resonant scattering

Ivan Troyan,[1,2*†] Alexander Gavriliuk,[2,3†] Rudolf Rüffer,[4] Alexander Chumakov,[4,5]
Anna Mironovich,[3] Igor Lyubutin,[2] Dmitry Perekalin,[6]
Alexander P. Drozdov,[1] Mikhail I. Eremets[1]



nature physics

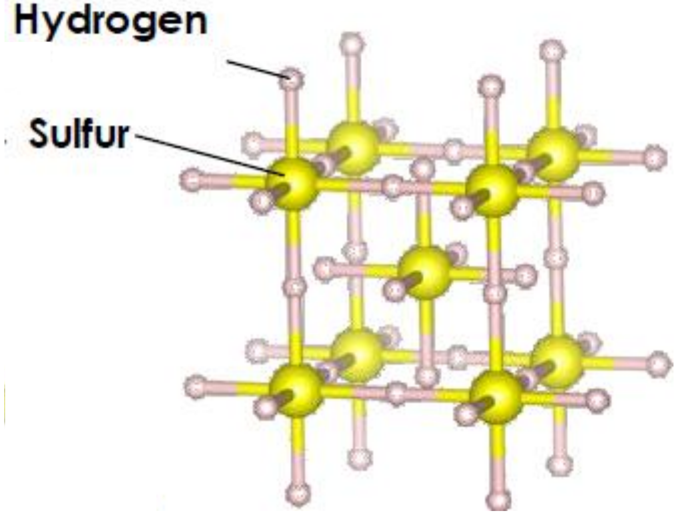
09 MAY 2016

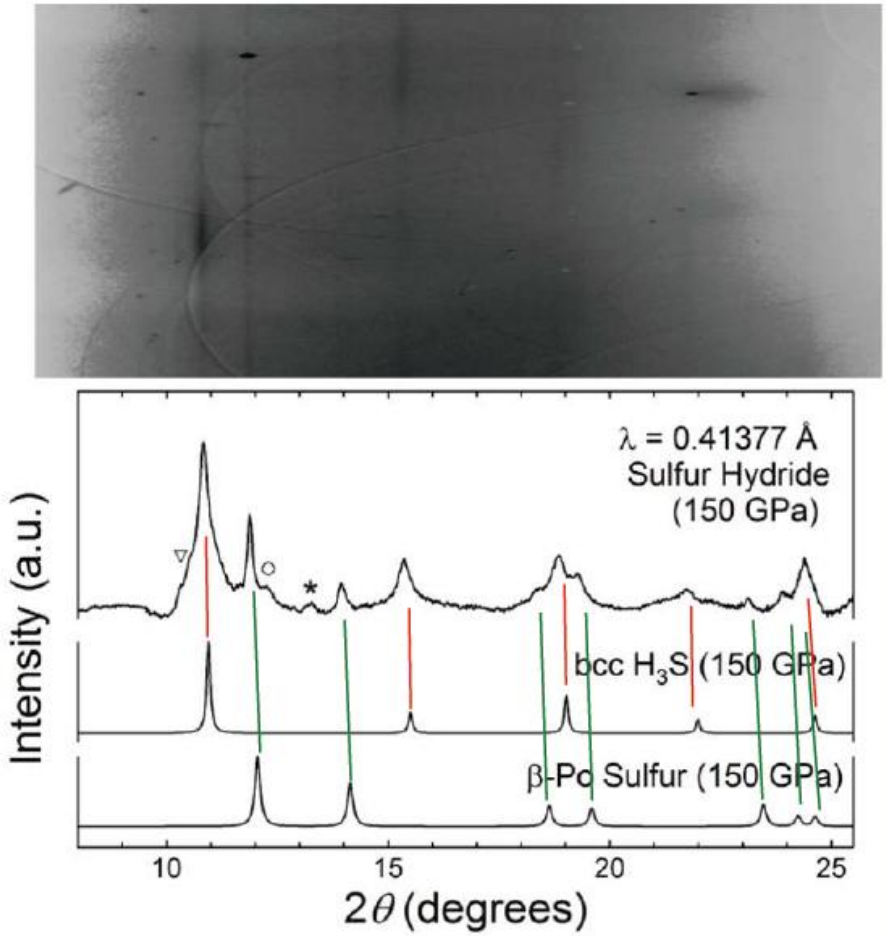
Crystal structure of the superconducting phase of sulfur hydride

Mari Einaga, Masafumi Sakata, Takahiro Ishikawa, Katsuya Shimizu, Mikhail I. Eremets, Alexander P. Drozdov, Ivan A. Troyan, Naohisa Hirao & Yasuo Ohishi

H_3S (bcc)

Im-3m





H_3S (bcc) + S (β-Po)

„Turning" Nitrogen into diamond

PHYSICAL REVIEW B VOLUME 46, NUMBER 22 1 DECEMBER 1992-II

Polymeric nitrogen

C. Mailhiot, L. H. Yang, and A. K. McMahan
Lawrence Livermore National Laboratory, University of California, Livermore, California 94551
(Received 22 April 1992; revised manuscript received 23 June 1992)

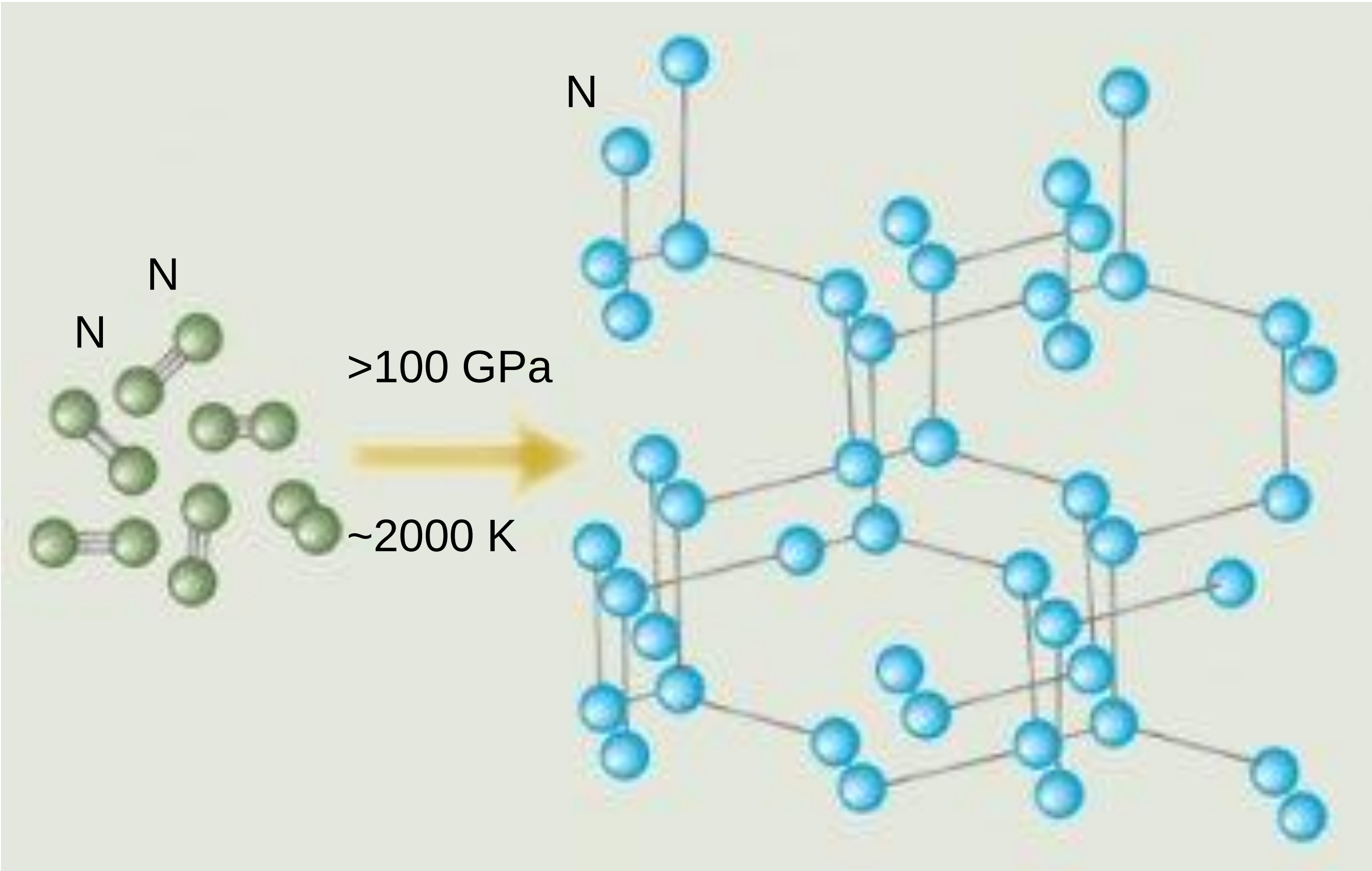
The equilibrium phase boundary between single-bonded, threefold-coordinated polymeric forms of nitrogen, and the observed, triple-bonded diatomic phases, is predicted to occur at relatively low (50 ± 15 GPa) pressure. This conclusion is based on extensive local-density-functional total-energy calculations for polymeric structures (including that of black phosphorus, and another with all *gauche* dihedral angles) and diatomic structures (including that of the observed high-pressure ε-N_2 phase). We believe the diatomic phase of nitrogen, observed up to 180 GPa and room temperature, to be metastable at these conditions, and that such hysteresis enhances the prospects for the existence of a metastable polymeric form of nitrogen at ambient conditions. In this regard, we show that the black-phosphorus and cubic *gauche* polymeric forms of nitrogen would encounter significant barriers along high-symmetry paths to dimerization at atmospheric pressure.

nature materials
04 JULY 2004

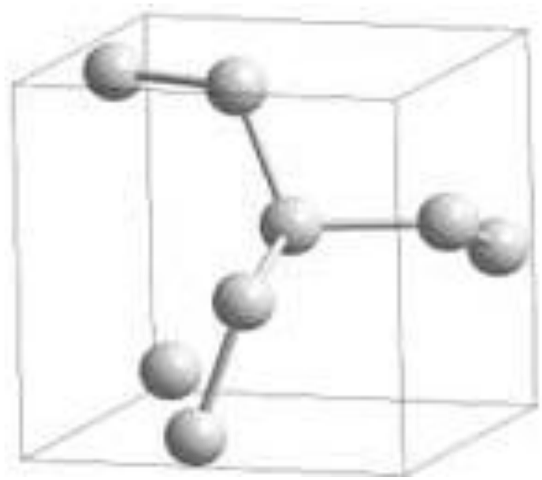
Single-bonded cubic form of nitrogen

MIKHAIL I. EREMETS[1*], ALEXANDER G. GAVRILIUK[1,2,3], IVAN A. TROJAN[1,3], DYMITRO A. DZIVENKO[1] AND REINHARD BOEHLER[1]

Polymeric cg-N structure: each nitrogen atom is connected to three neighbours by three single covalent bonds.



Primitive cell



Cubic gauch (cg- N)

$I2_13$

a **triple** bond
~ 225 kcal/mol

a **single** bond
~ 40 kcal/mol

PHYSICAL REVIEW LETTERS

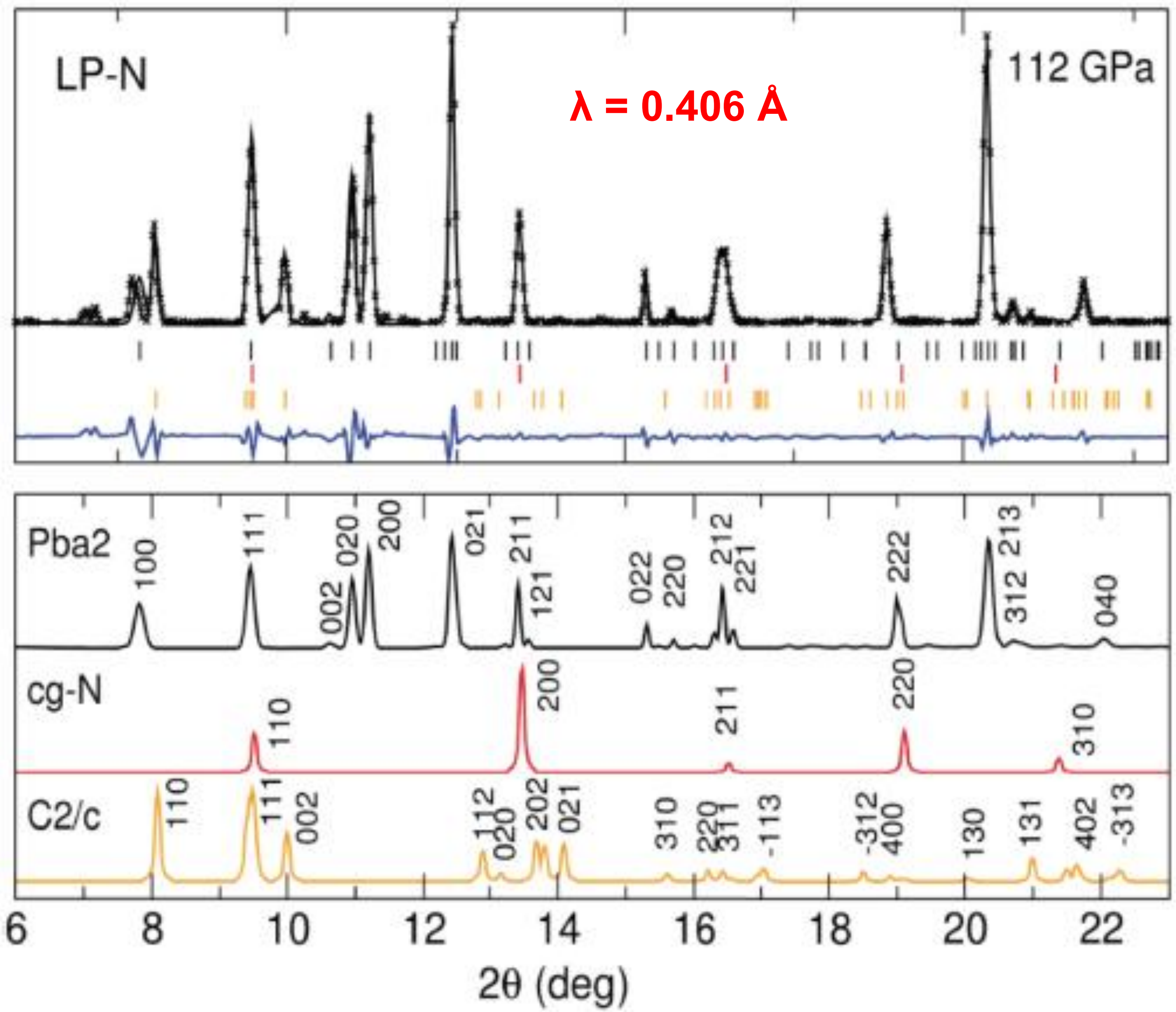
Pressure-Induced Symmetry-Lowering Transition in Dense Nitrogen to Layered Polymeric Nitrogen (LP-N) with Colossal Raman Intensity

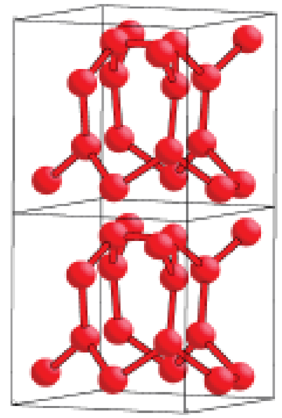
PRL **113**, 205502 (2014)

Dane Tomasino,[1] Minseob Kim,[1] Jesse Smith,[2] and Choong-Shik Yoo[1,*]

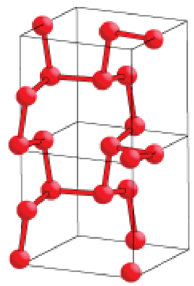
Synthesis conditions

Pressure: 126 – 175 GPa; Temperature ~ 3000 K

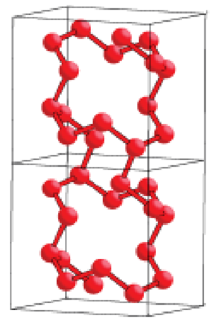




Pba2-N_7



I$2_1$3-N_{10} (cg- N)



*C*2/*c*-N_{12}

New „taste”of chemistry

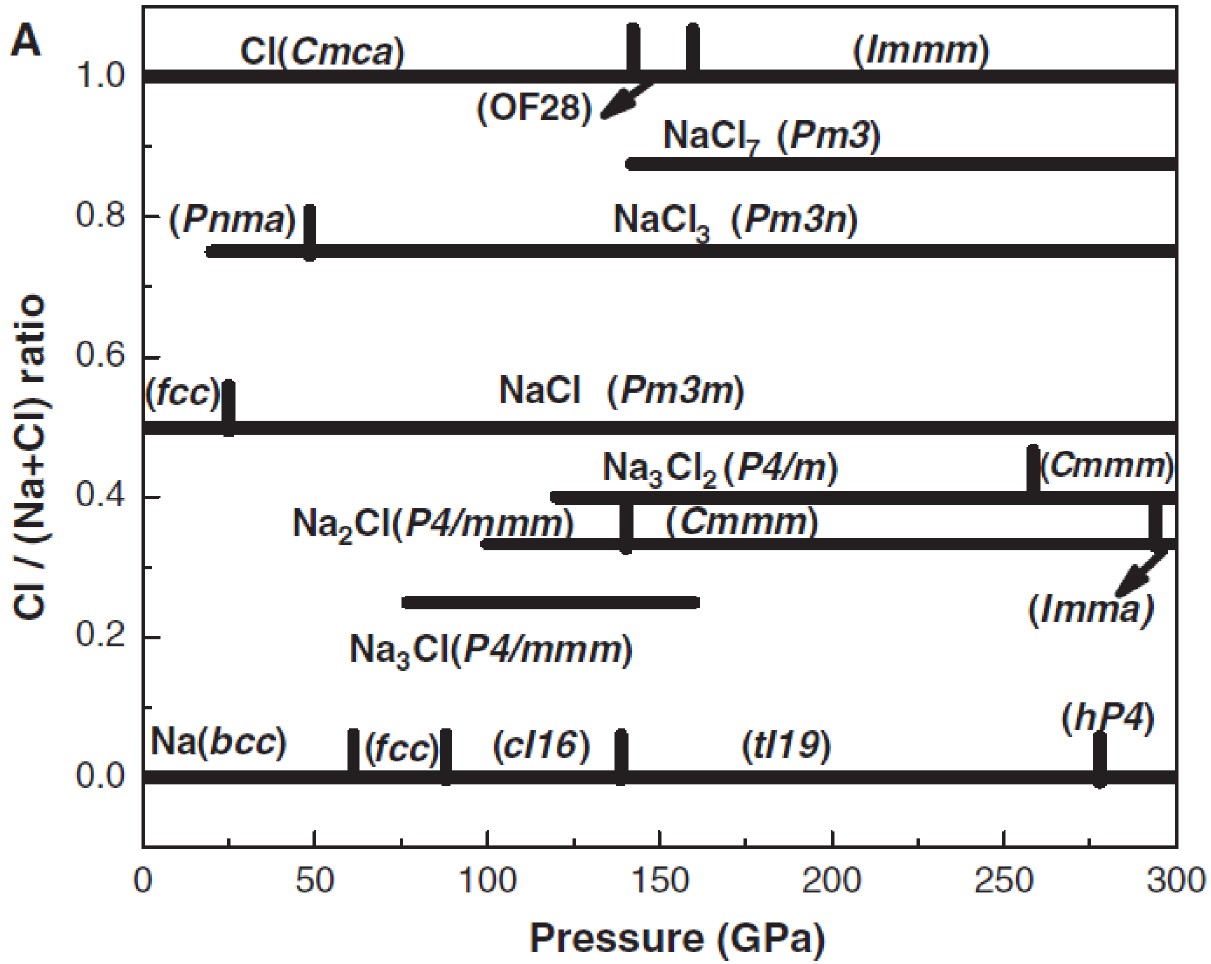
Science AAAS

20 DECEMBER 2013

Unexpected Stable Stoichiometries of Sodium Chlorides

Weiwei Zhang,[1,2]*† Artem R. Oganov,[2,3,4]*† Alexander F. Goncharov,[5,6] Qiang Zhu,[2] Salah Eddine Boulfelfel,[2] Andriy O. Lyakhov,[2] Elissaios Stavrou,[5] Maddury Somayazulu,[5] Vitali B. Prakapenka,[7] Zuzana Konôpková[8]

THEORY



Science AAAS
20 DECEMBER 2013

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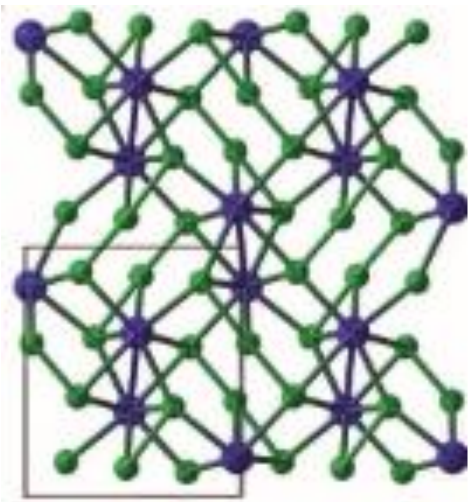
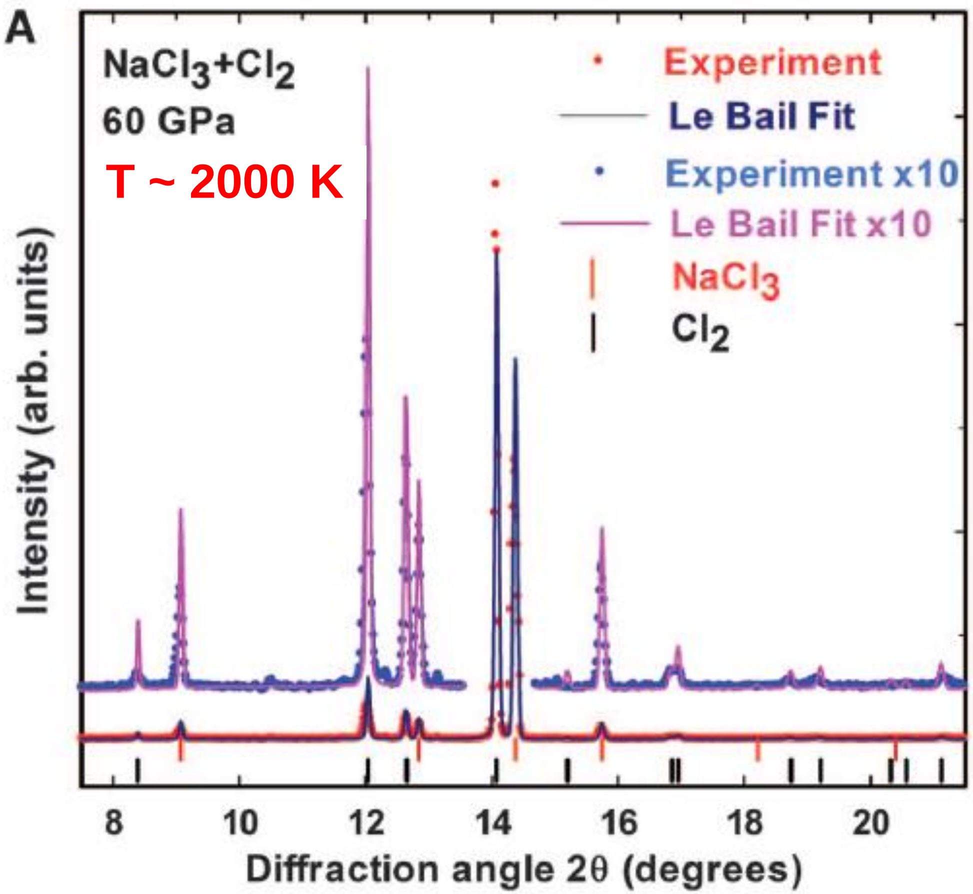
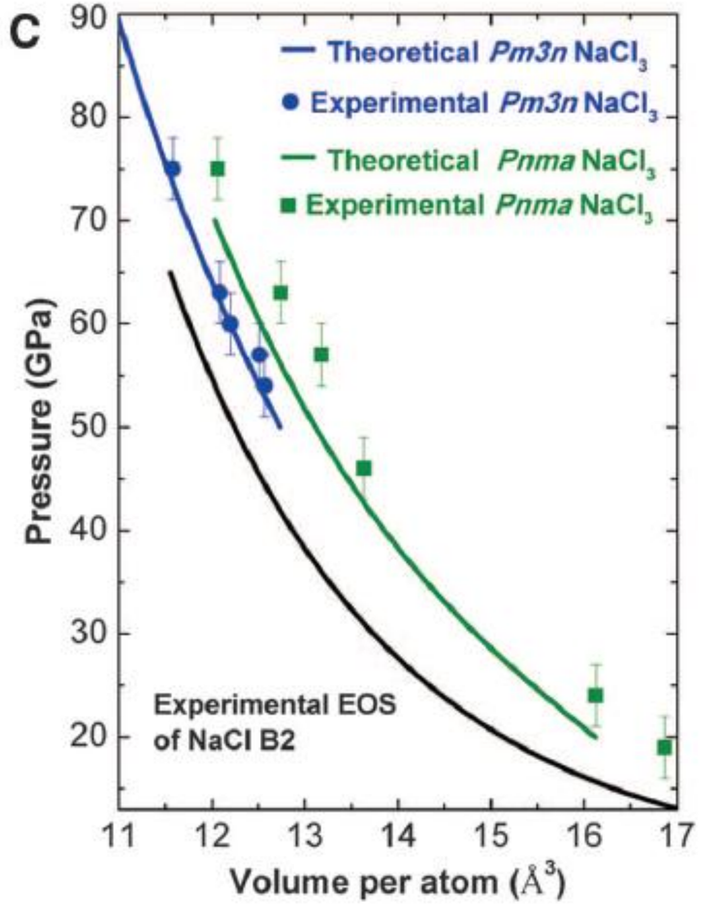
EXPERIMENT

$NaCl_3$

Na Cl







λ = 0.5146 Å

Science AAAS

20 DECEMBER 2013

Unexpected Stable Stoichiometries of Sodium Chlorides

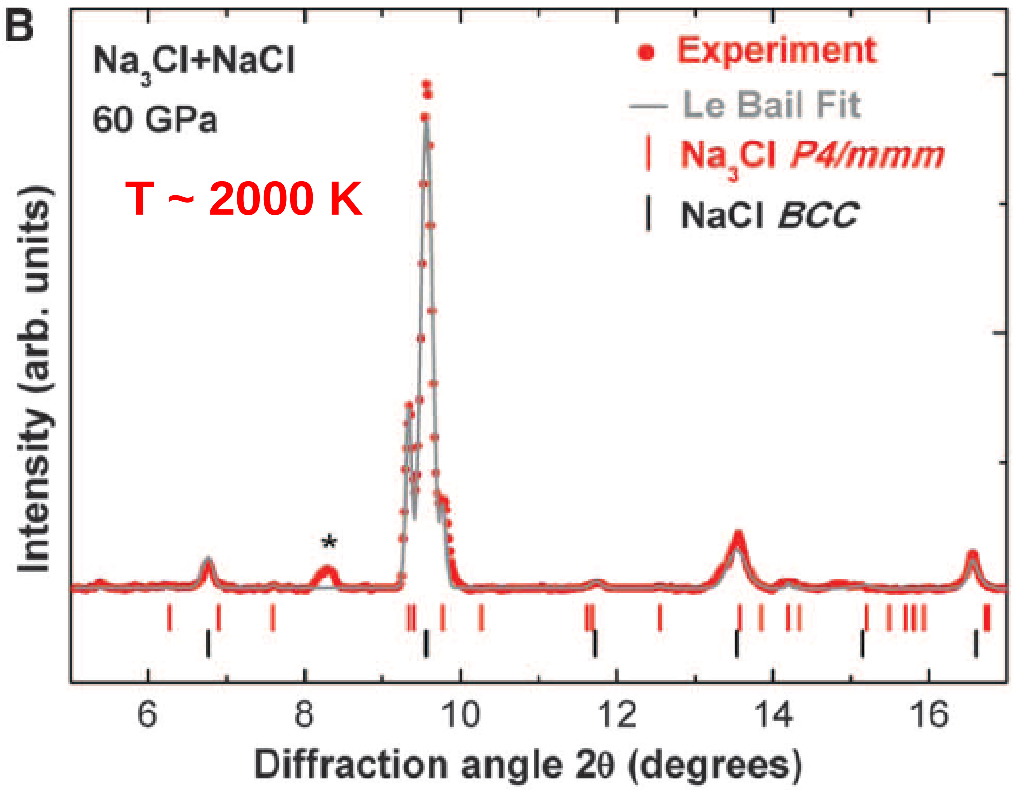
Weiwei Zhang,[1,2]*† Artem R. Oganov,[2,3,4]*† Alexander F. Goncharov,[5,6] Qiang Zhu,[2] Salah Eddine Boulfelfel,[2] Andriy O. Lyakhov,[2] Elissaios Stavrou,[5] Maddury Somayazulu,[5] Vitali B. Prakapenka,[7] Zuzana Konôpková[8]

EKSPERYMENT

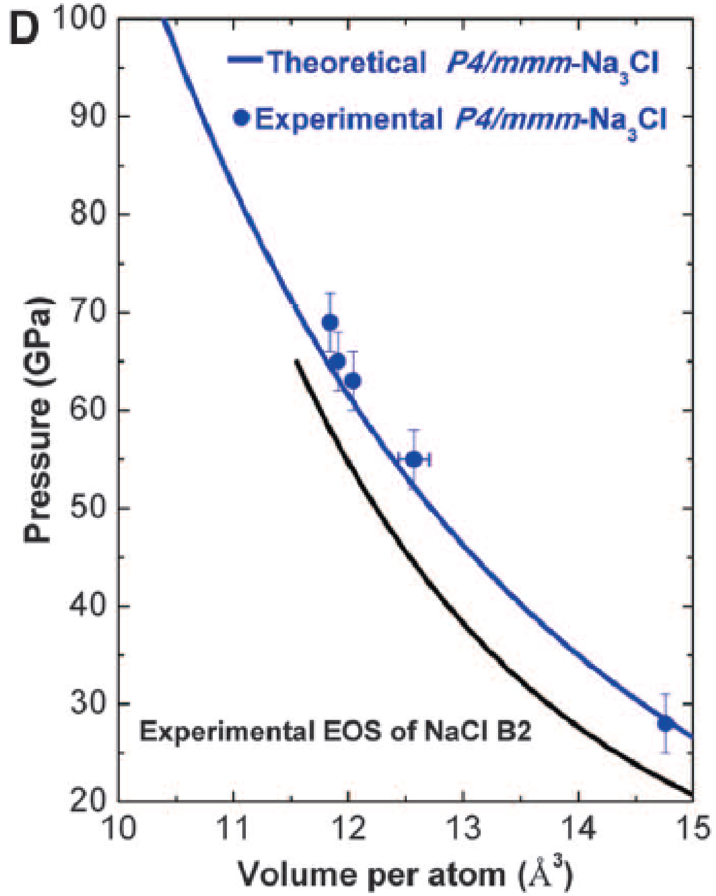
Na_3Cl

Cl

Na



λ = 0.3344 Å



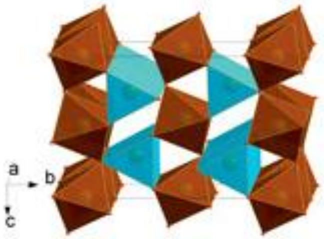
„Ground”-breaking news

nature COMMUNICATIONS

Structural complexity of simple Fe_2O_3 at high pressures and temperatures

11 FEBRUARY 2016

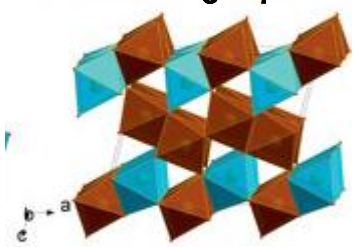
Hematite
Fe_2O_3



Cmcm

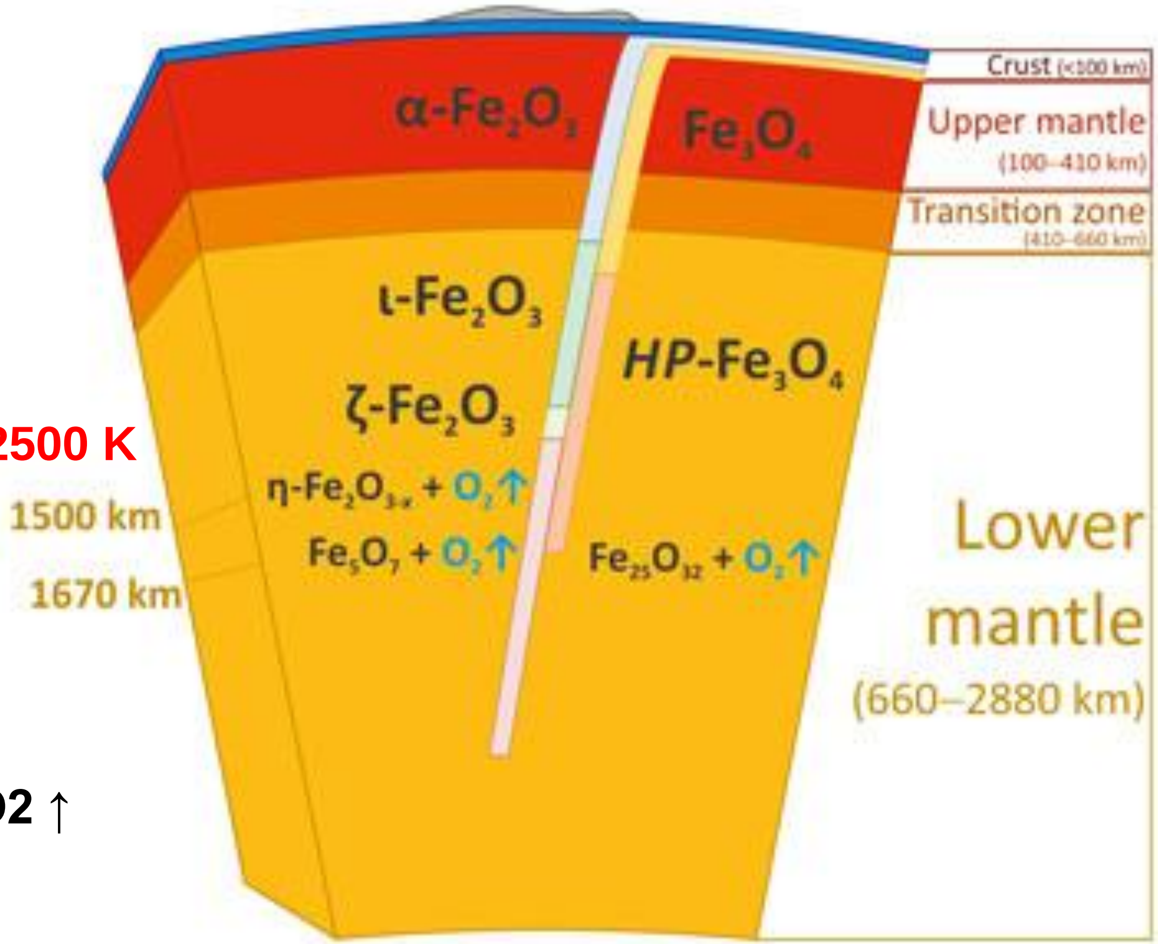
~ 60 GPa   2000 – 2500 K

Fe_5O_7

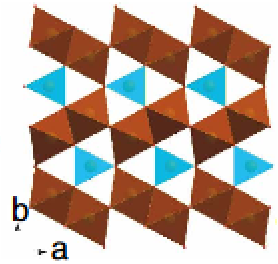


+ O2 ↑

C2/m



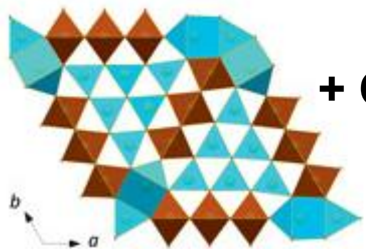
Magnetite
Fe_3O_4
($FeO + Fe_2O_3$)



Bbmm

2000 –2500 K   ~70 GPa

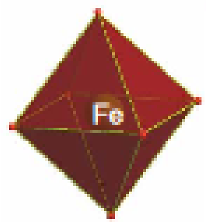
$Fe_{25}O_{32}$



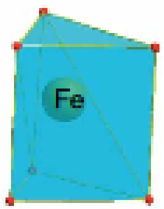
+ O2 ↑

C2/m

Building blocks:



FeO_6 octahedra



FeO_6 trigonal prism

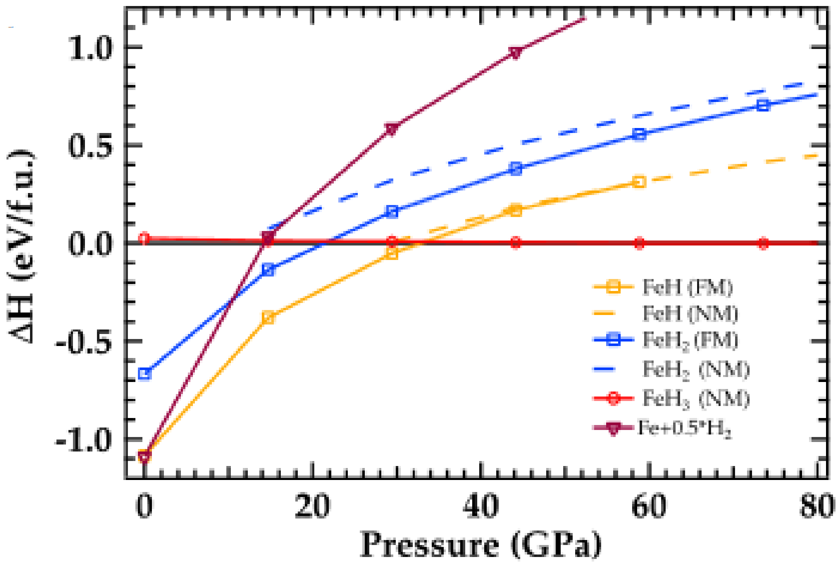
PHYSICAL REVIEW LETTERS

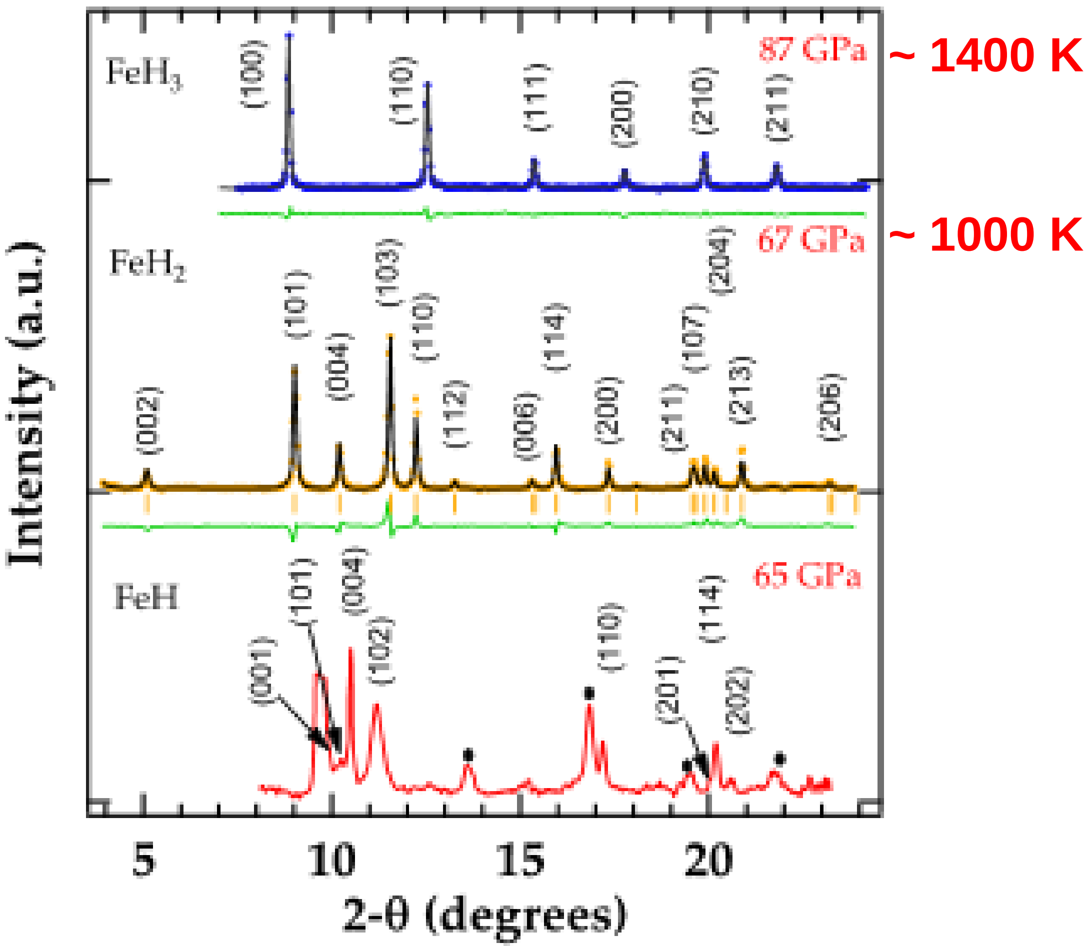
PRL **113**, 205502 (2014)

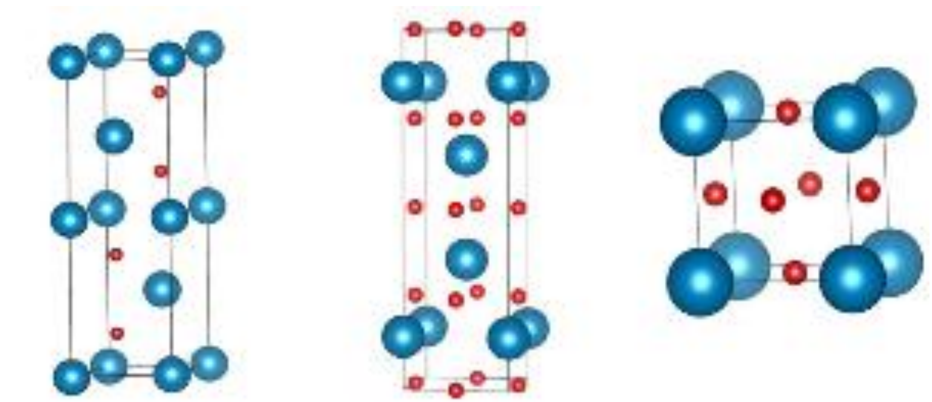
New Iron Hydrides under High Pressure

Charles M. Pépin,* Agnès Dewaele, Grégory Geneste, and Paul Loubeyre†

Mohamed Mezouar







dhcp-FeH ($P6_3/mmc$) FeH$_2$ ($I4/mmm$) FeH$_3$ ($Pm\text{-}3m$)

„This is but the least
we have yet seen of the work of the Lord,
much is still hidden from us”

Carl Linnaeus

Quest for record pressure

nature COMMUNICATIONS

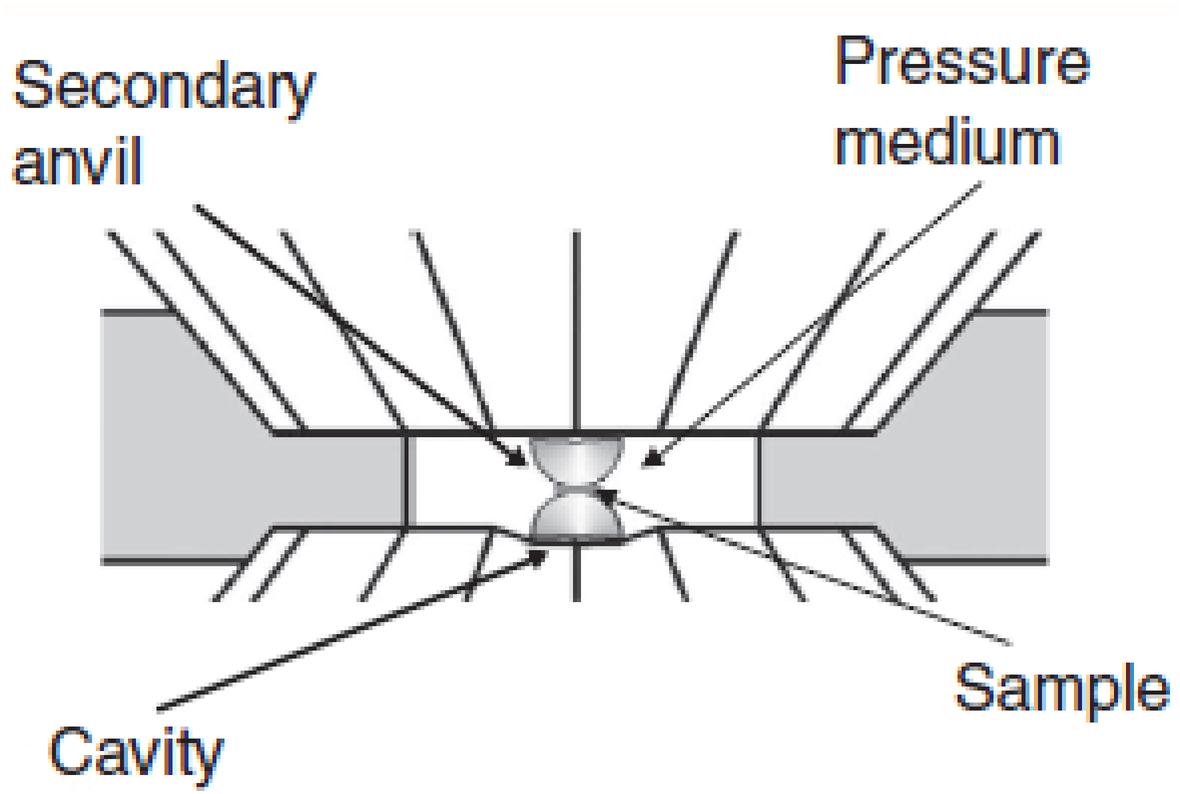
ARTICLE

Received 30 Apr 2012 | Accepted 3 Sep 2012 | Published 23 Oct 2012

DOI: 10.1038/ncomms2160

Implementation of micro-ball nanodiamond anvils for high-pressure studies above 6 Mbar

Leonid Dubrovinsky[1,*], Natalia Dubrovinskaia[2,*], Vitali B. Prakapenka[3] & Artem M. Abakumov[4]



ARTICLE
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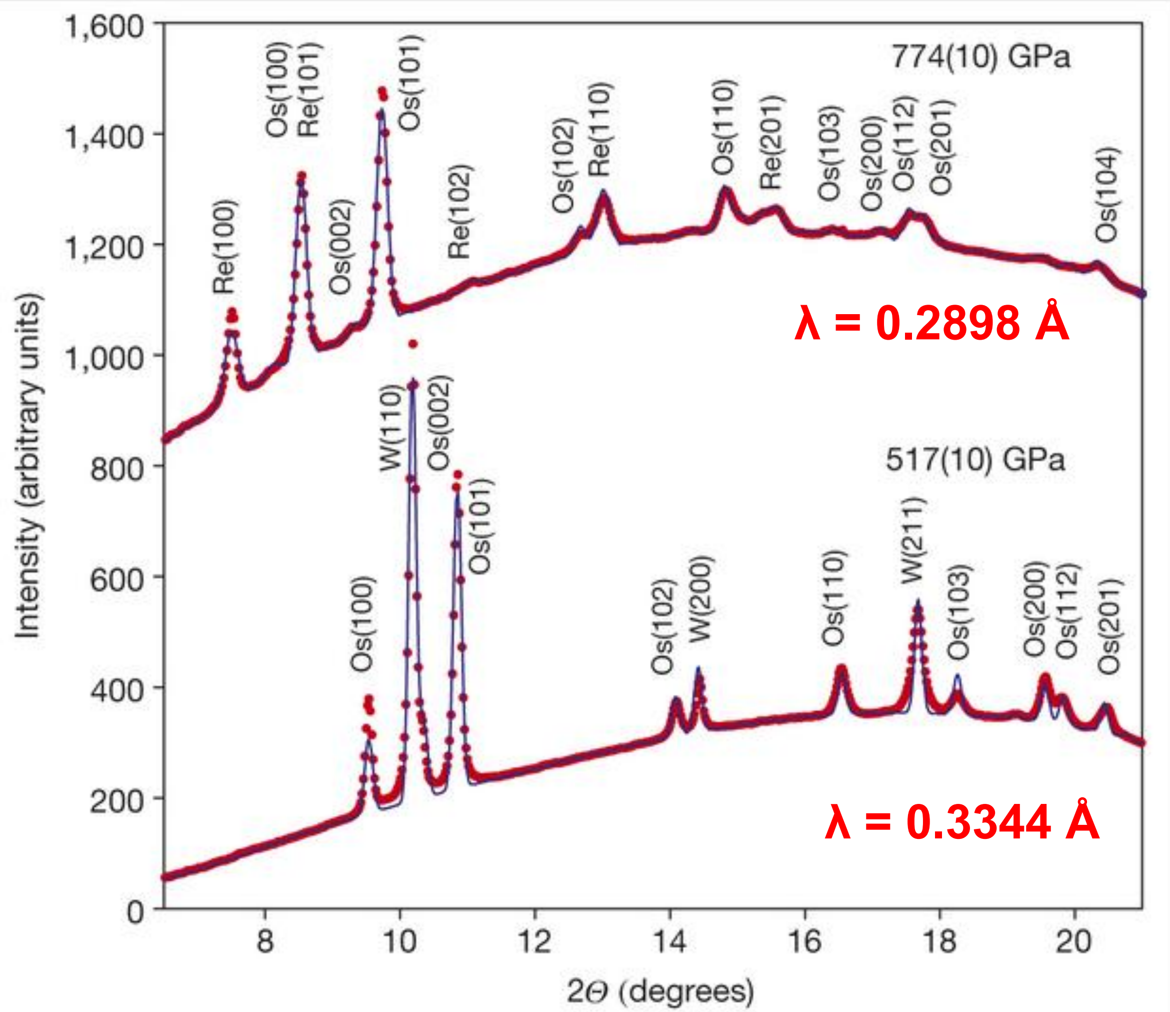
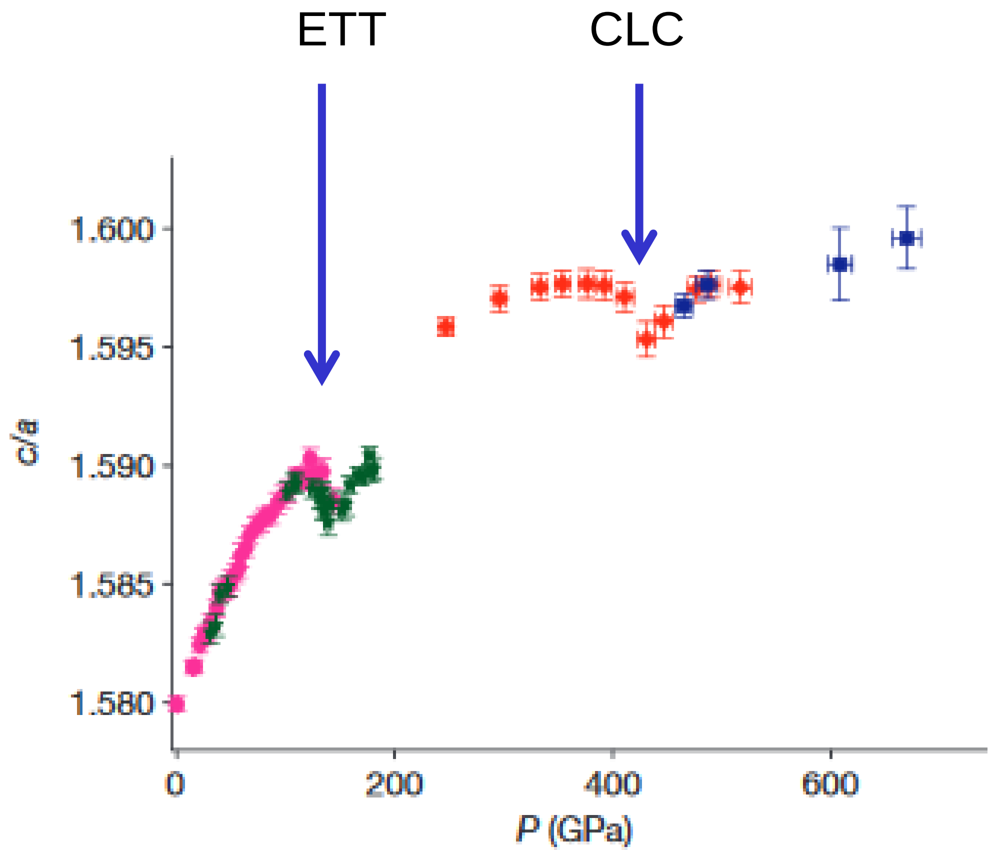
Implementation of micro-ball nanodiamond anvils for high-pressure studies above 6 Mbar

Leonid Dubrovinsky[1,*], Natalia Dubrovinskaia[2,*], Vitali B. Prakapenka[3] & Artem M. Abakumov[4]

Osmium





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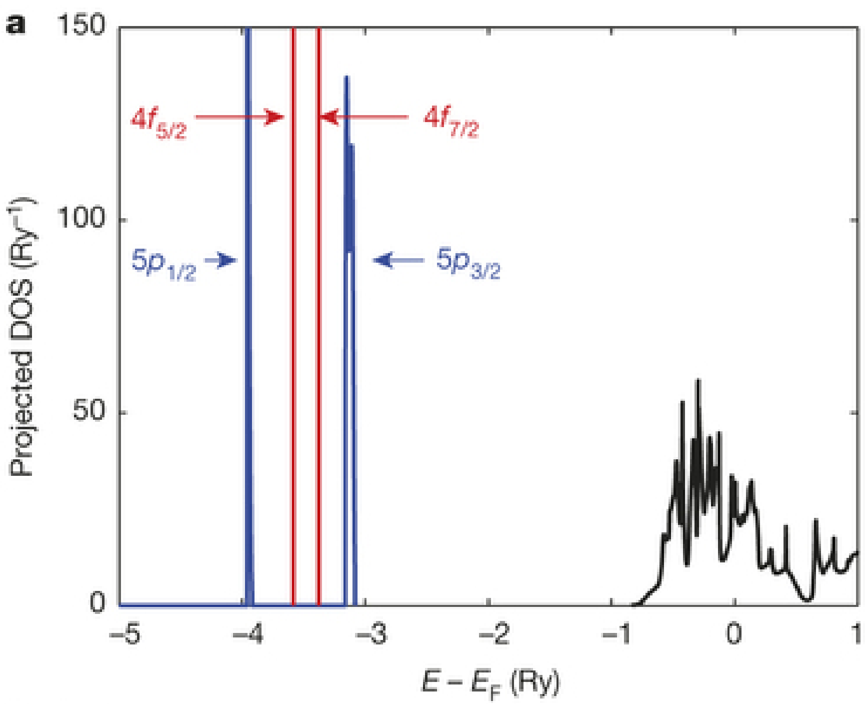
Implementation of micro-ball nanodiamond anvils for high-pressure studies above 6 Mbar

Leonid Dubrovinsky[1,*], Natalia Dubrovinskaia[2,*], Vitali B. Prakapenka[3] & Artem M. Abakumov[4]

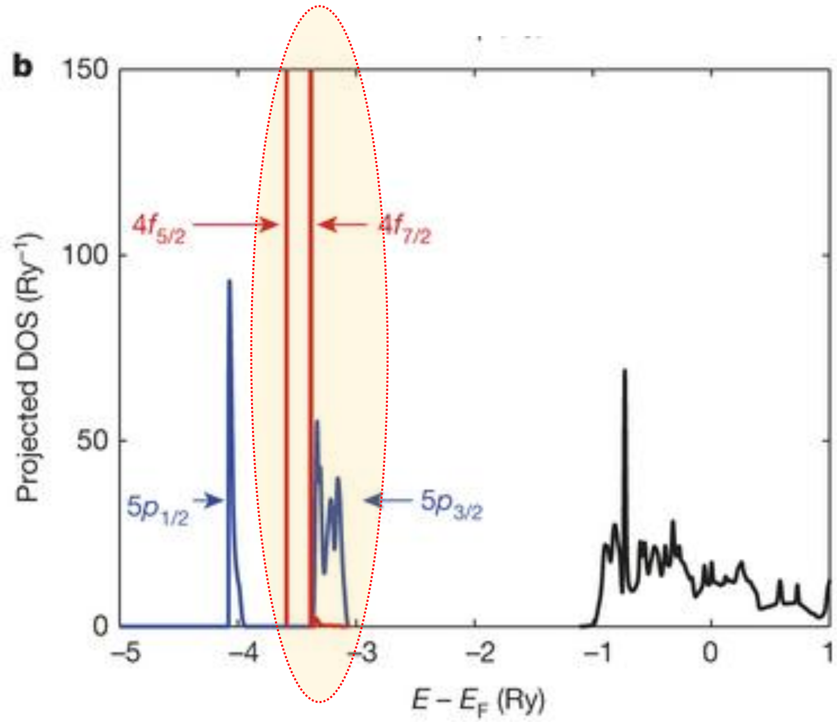
Osmium

Core-Level Crossing (CLC)

0 GPa



396 GPa

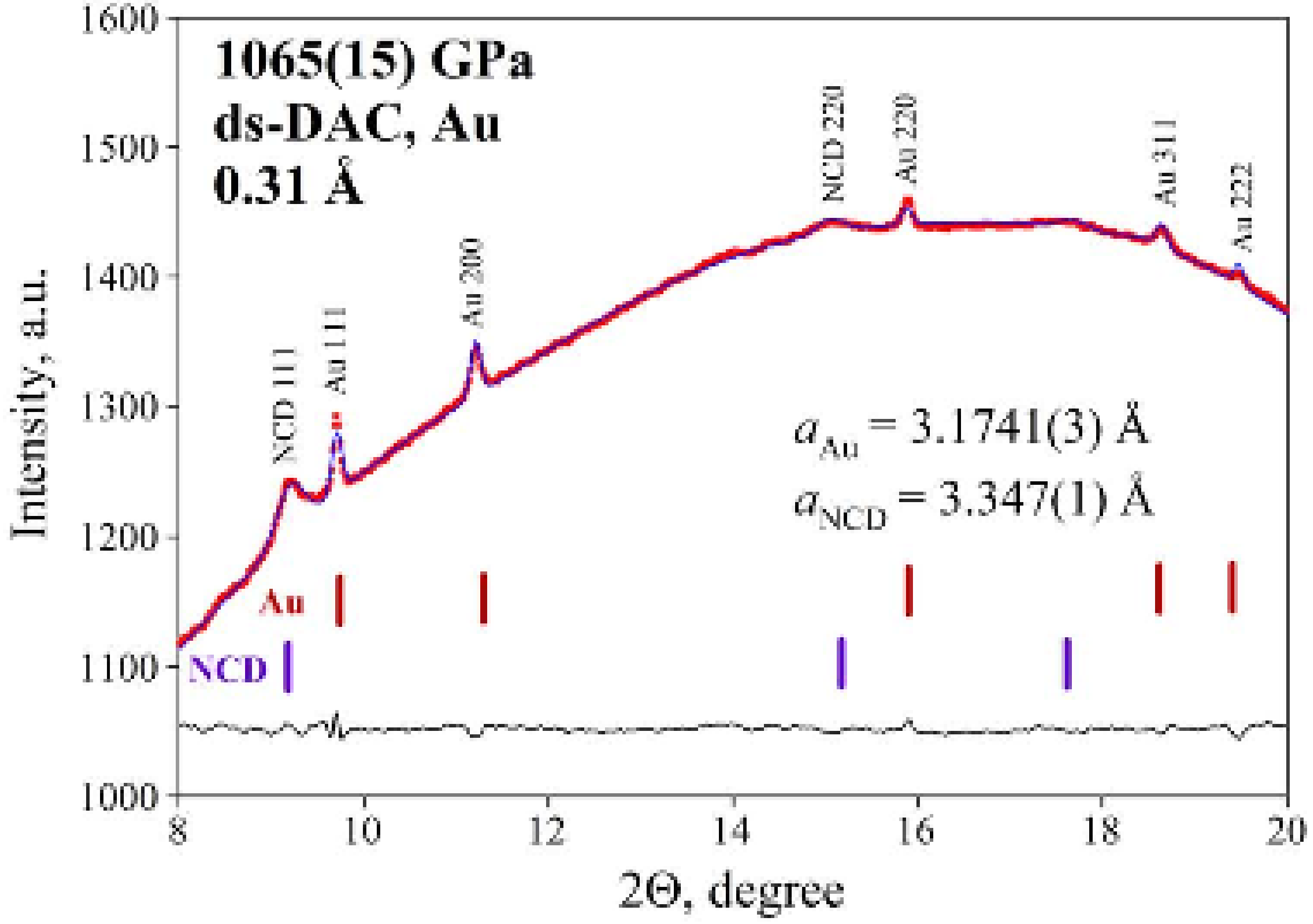


ScienceAdvances
AAAS

Terapascal static pressure generation with ultrahigh yield strength nanodiamond

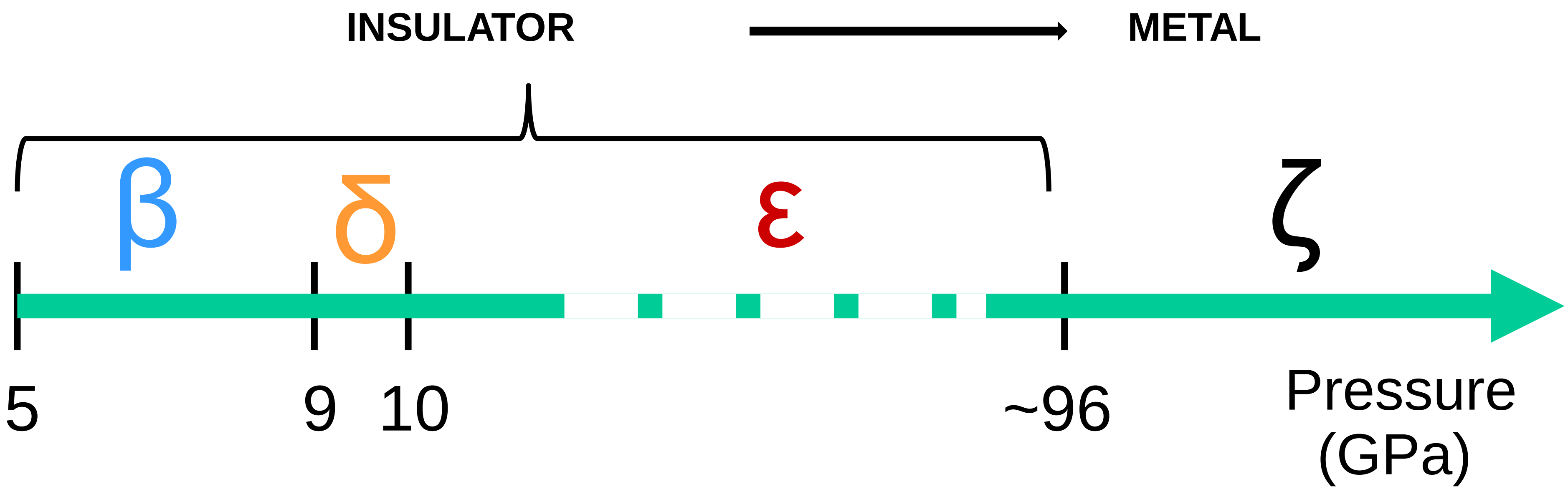
Natalia Dubrovinskaia, Leonid Dubrovinsky, Natalia A. Solopova, Artem Abakumov, Stuart Turner, Michael Hanfland, Elena Bykova, Maxim Bykov, Clemens Prescher, Vitali B. Prakapenka, Sylvain Petitgirard, Irina Chuvashova, Biliana Gasharova, Yves-Laurent Mathis, Petr Ershov, Irina Snigireva and Anatoly Snigirev (July 20, 2016)

Sci Adv 2016, 2:.
doi: 10.1126/sciadv.1600341



✓ Oxygen

Becomes **Solid** under pressure > 50 000 atm (5GPa)
Becomes **Metal** under pressure > 960 000 atm (96 GPa)



Under pressure a number of spectacular phase transformations (color change) can be observed in oxygen.