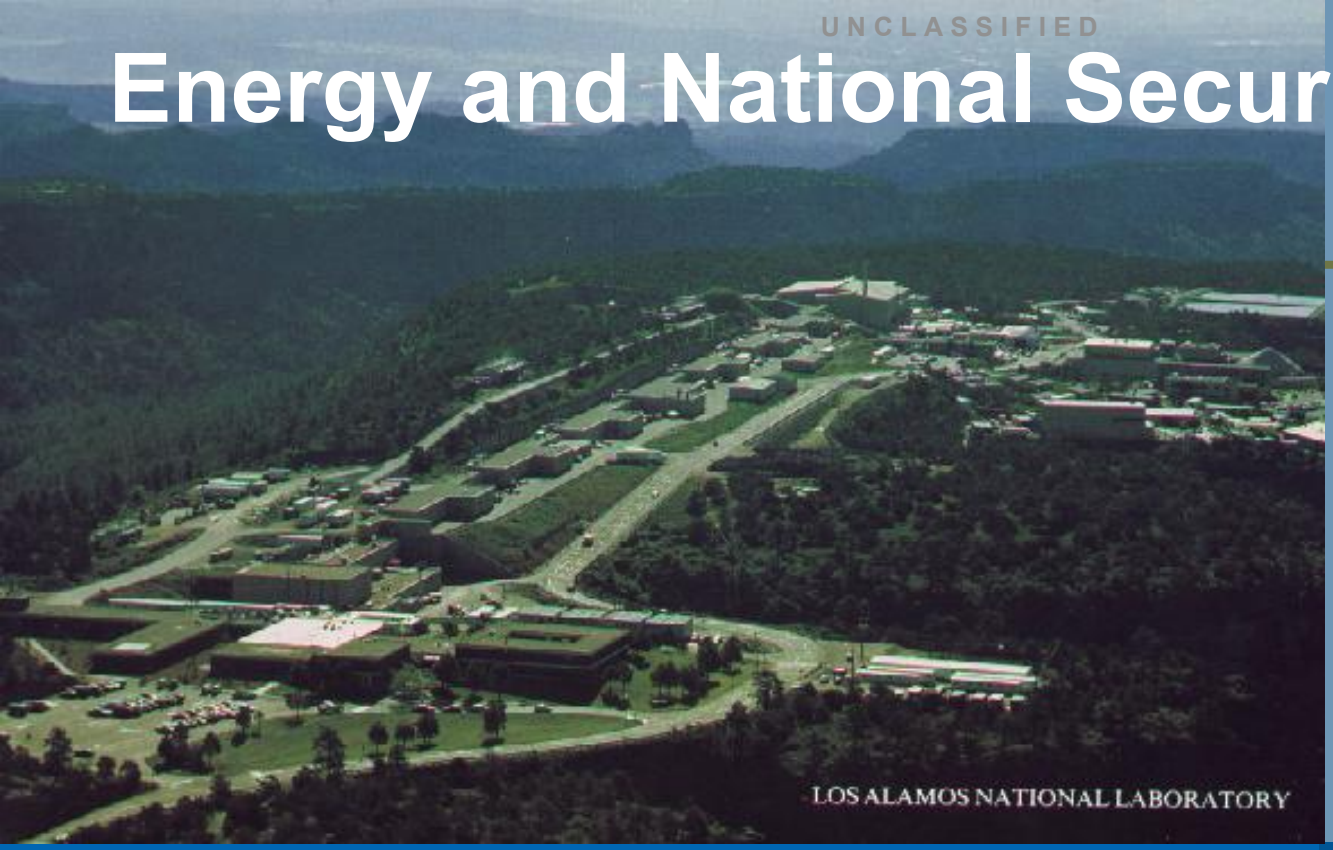
Energy and National Security Research at LANSCE



Stewardship Fellows Conference
Krell Institute & NNSA, *Washington DC*
June 21-22, 2010

Alan J. Hurd
Director, Lujan Neutron Scattering Center
LA-UR 10-03862

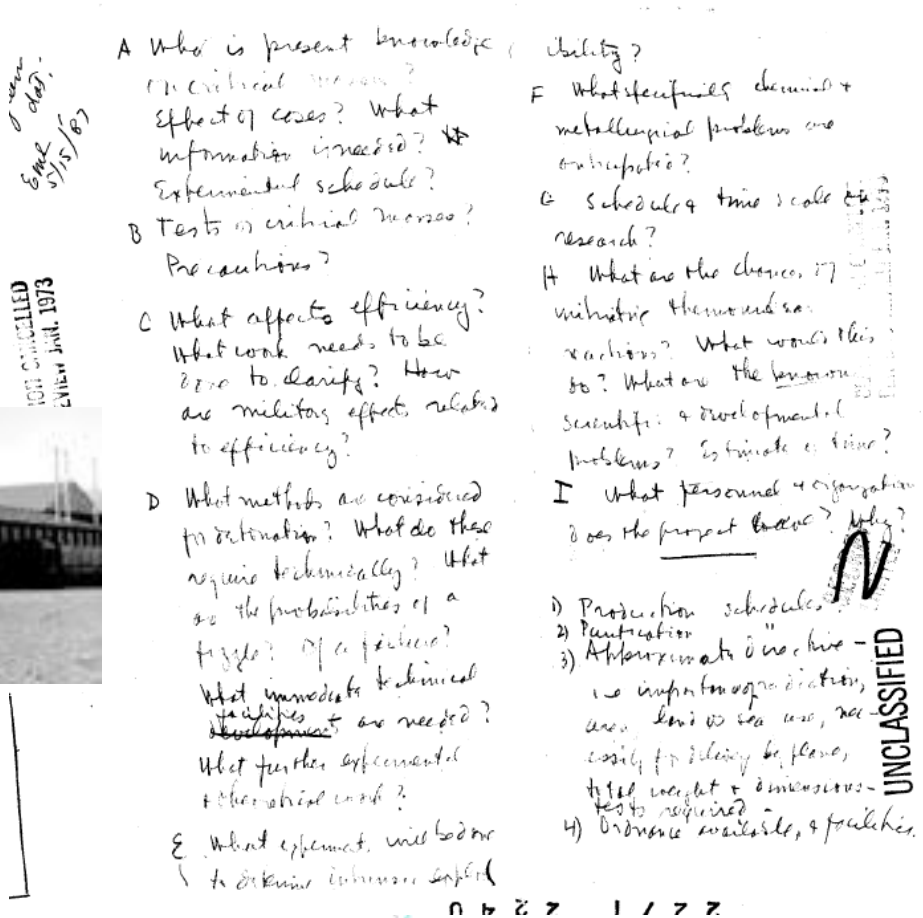
Los Alamos NATIONAL LABORATORY EST.1943
The World's Greatest Science Protecting America

Quick Poll

Who is the greatest living person?

1943
Oppenheimer designs Project Y on scrap of paper

Headquarters



1944 Manhattan


Rosen


Oppenheimer


Bethe


Feynman


Ulam

Bartlett


Groves


Fermi


Wilson


Metropolis


Agnew


Teller


Tuck


Los Alamos NATIONAL LABORATORY EST. 1943

LUJAN CENTER

Following Oppie's blueprint, accelerator-based experiments came to Los Alamos

A. What is present knowledge of critical masses?...

B. Tests of critical masses? Precautions?

C. What affects efficiency?...

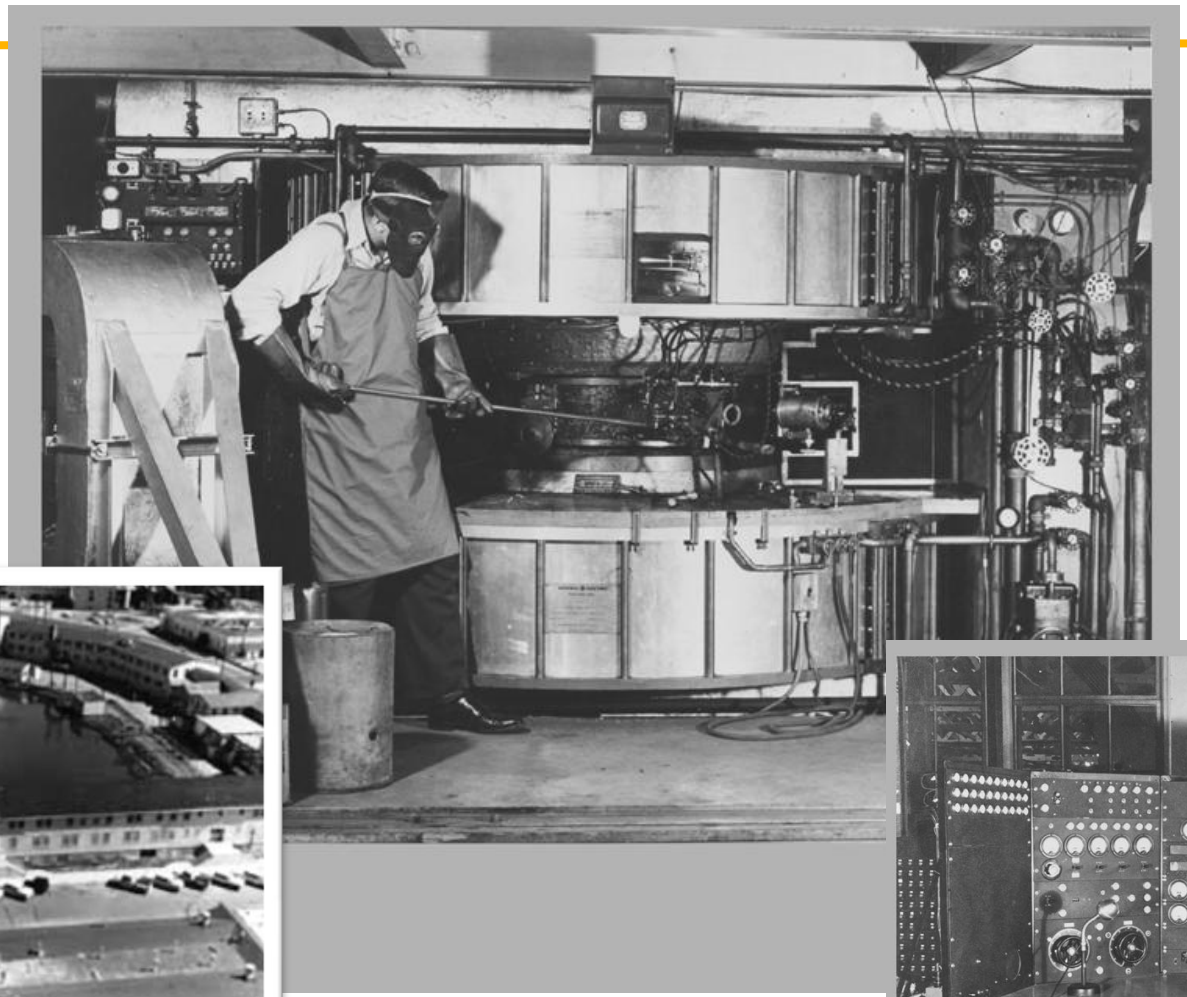
Hymer Friedell?, Robert R. Wilson[from Princeton], Percy Bridgeman[depart. chair] discussion of taking cyclotron to unkown destination

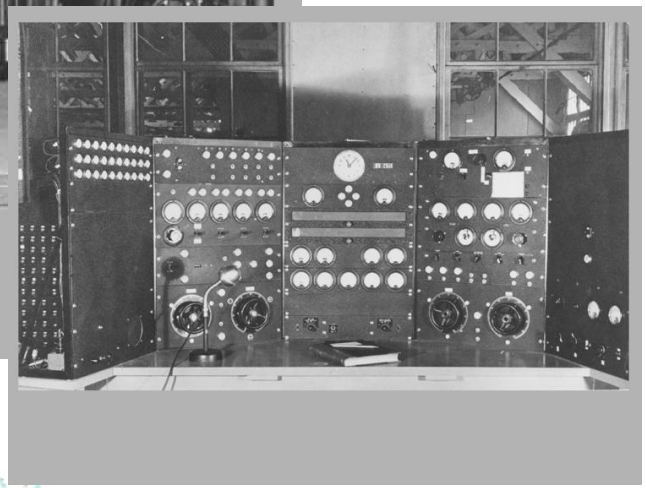
A What is present knowledge of critical masses? Effect of cases? What information is needed? Experimental schedule?

B Tests of critical masses? Precautions?

C What affects efficiency? What work needs to be done to clarify? How are military effects related to efficiency?

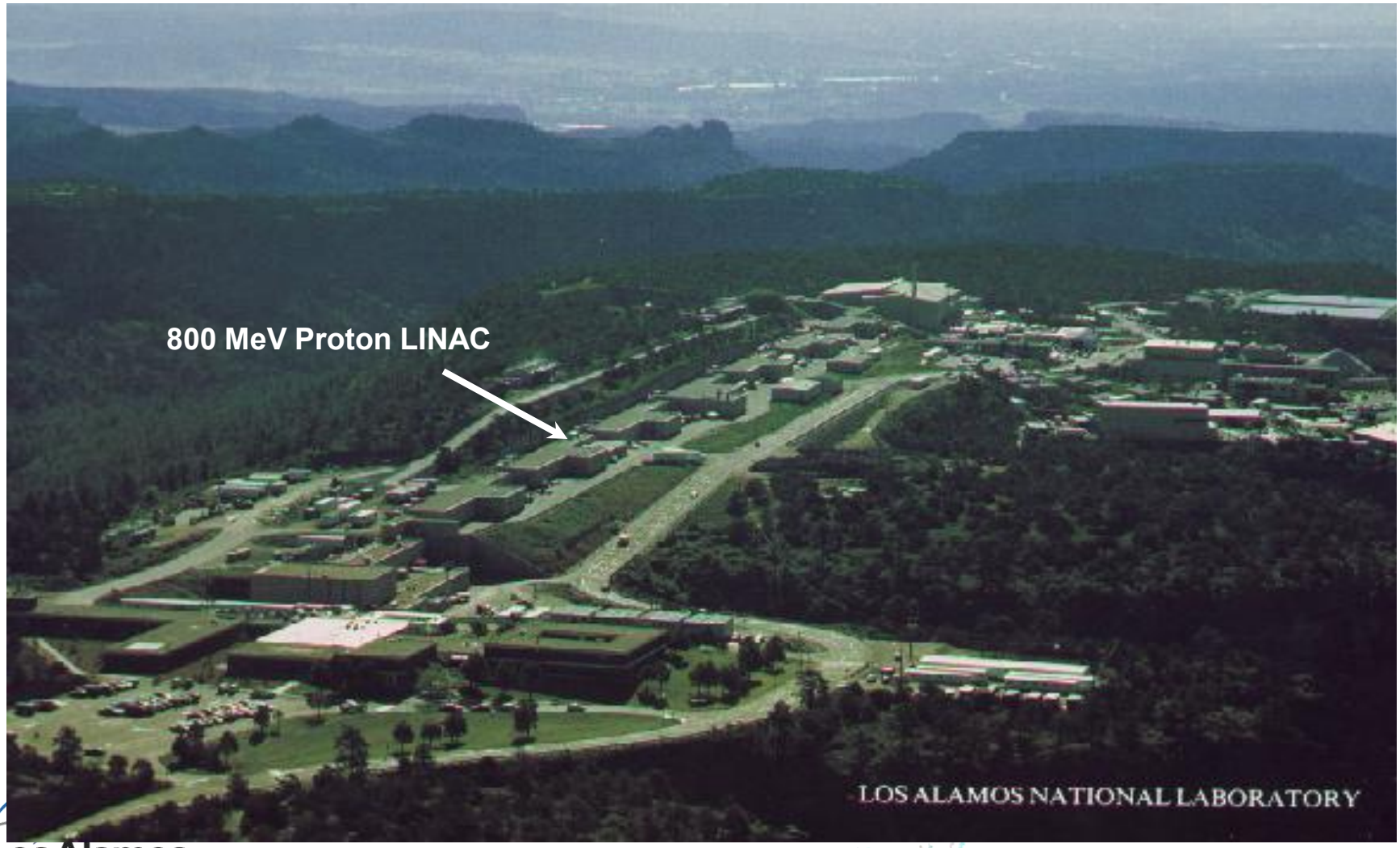
Rosen “rewarded himself” after the war by doing research on the Harvard Cyclotron in 1945





1976
LAMPF operations

LANSCE is a Megawatt Class accelerator
The backbone for future MaRIE*



Los Alamos NATIONAL LABORATORY EST. 1943

*Matter-Radiation Interactions in Extremes

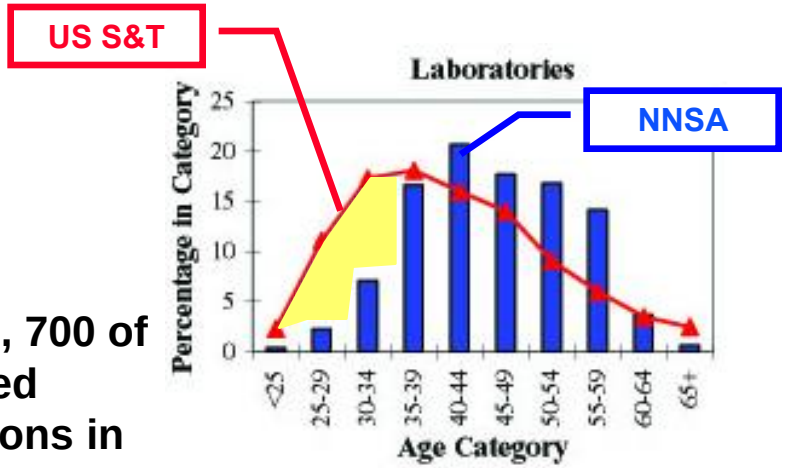
LANSCE Los Alamos Neutron Science Center

NNSA

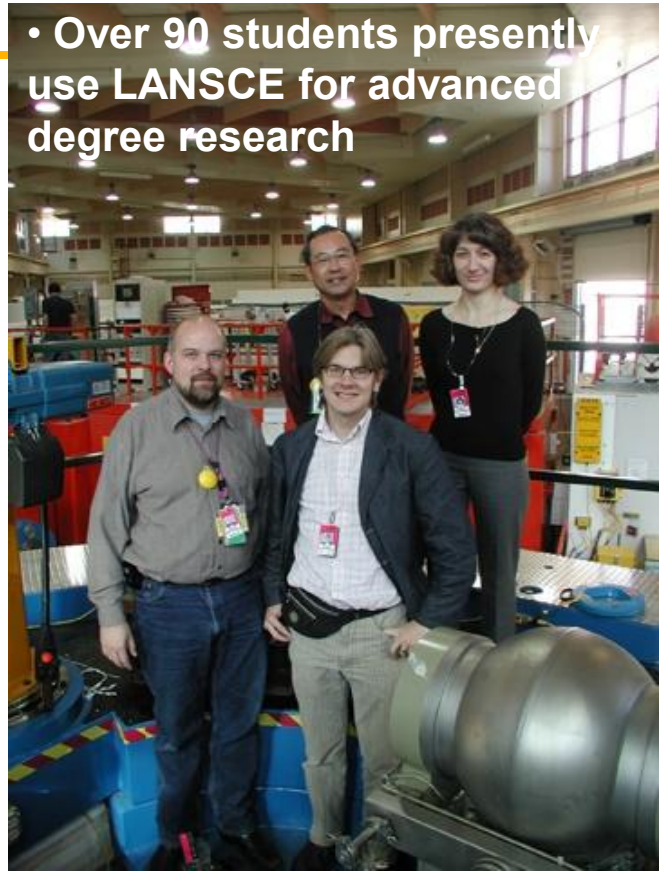
LANSCE provides a window to LANL

Over 300 LANSCE PhD theses 1972-2009

About 10% of Laboratory technical staff (n > 1200) have joined Los Alamos as a result of LAMPF or LANSCE based research



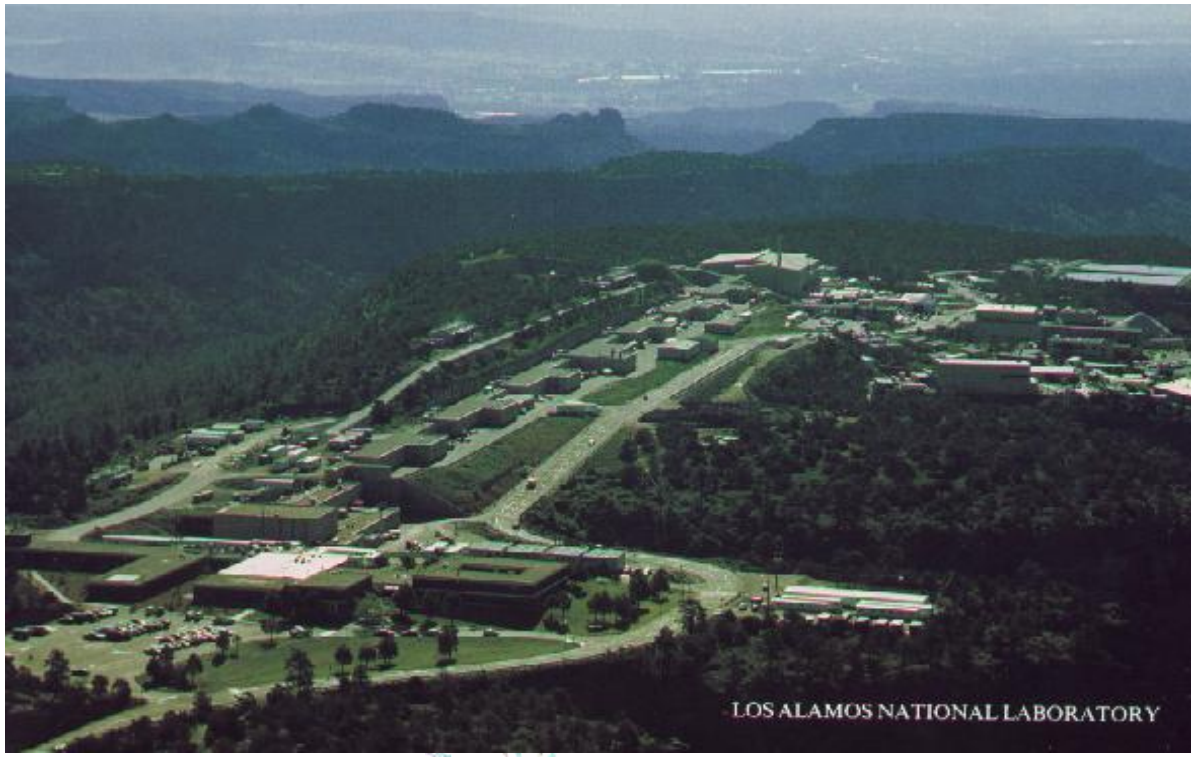
From 1981-2009, 700 of those have joined other organizations in the Laboratory, helping fill yellow gap



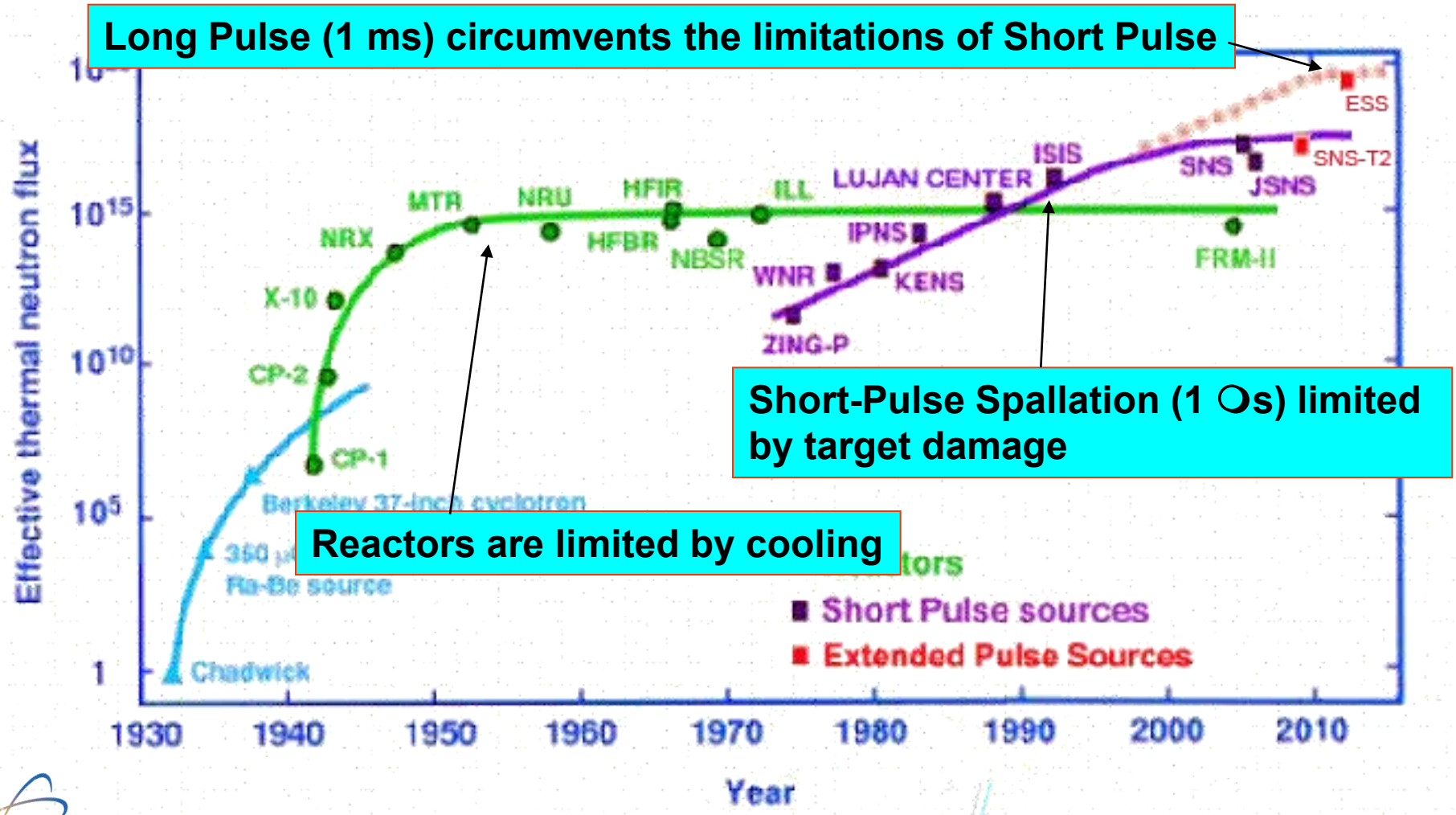
2005

Outline

- **Making neutrons**
- Using neutrons and why
- User Facilities
- Success stories



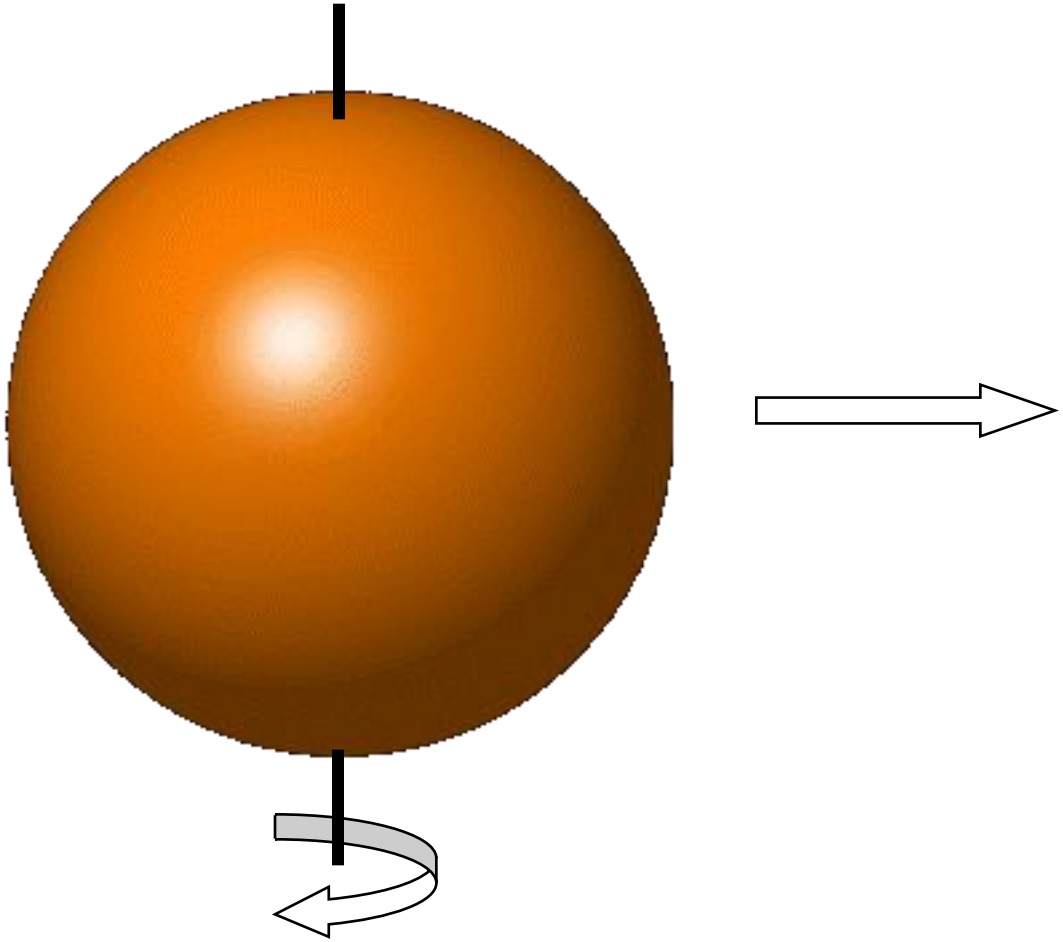
Spallation: now and future neutron sources



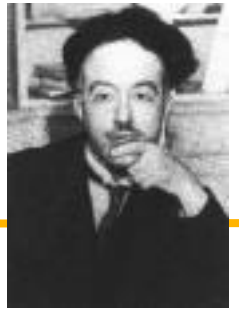
Outline

- Making neutrons
- **Using neutrons and why**
- User Facilities
- Success stories

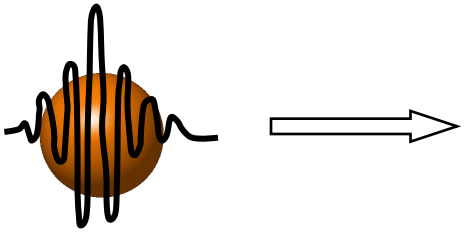
The neutron has mass, velocity and magnetism (spin)

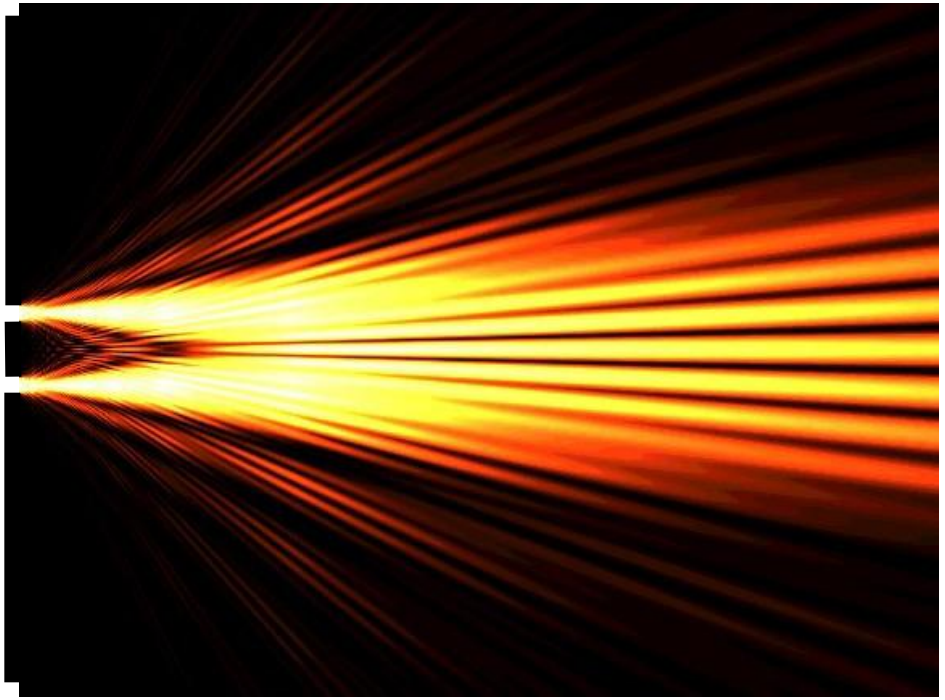


A moving neutron is wavelike

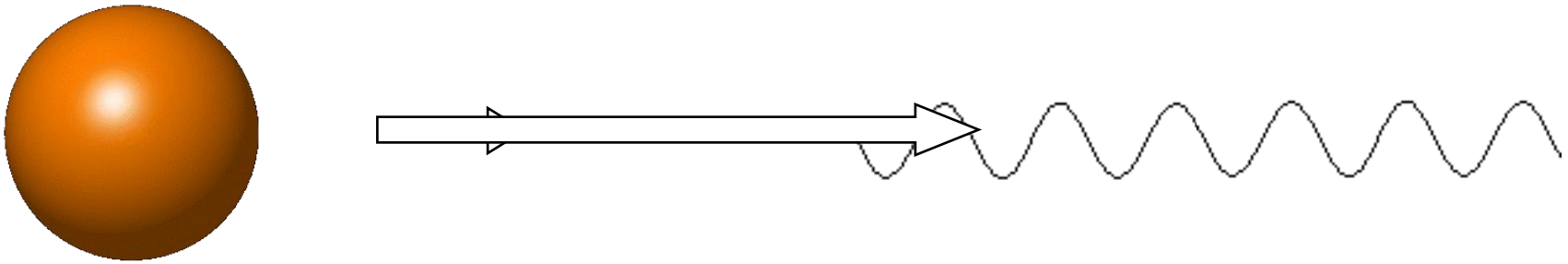


Louis de Broglie





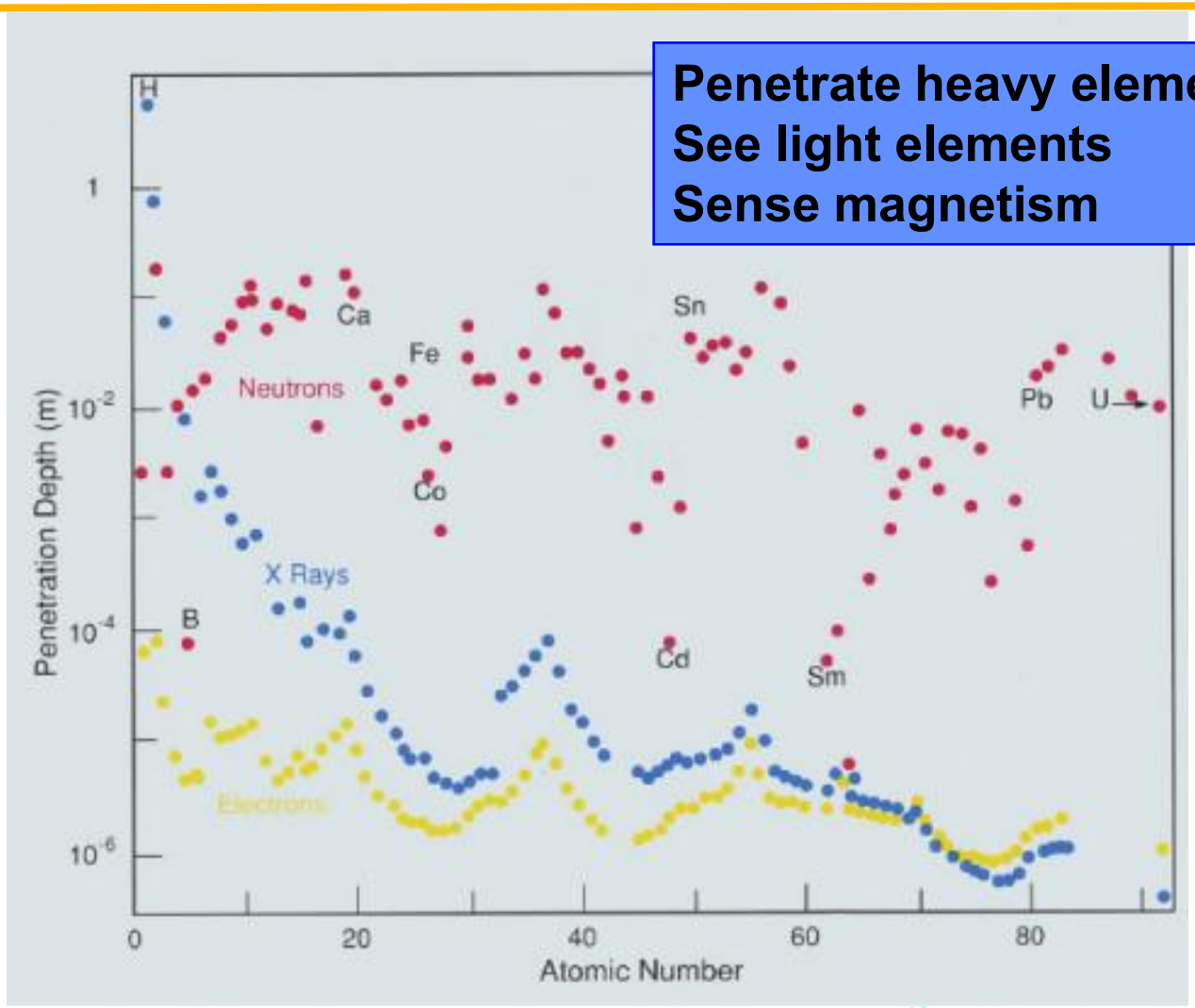
For materials science, cold and warm neutrons are required.



Fast

Slow = “Cold”

Why use neutrons?



Penetrate heavy elements
See light elements
Sense magnetism

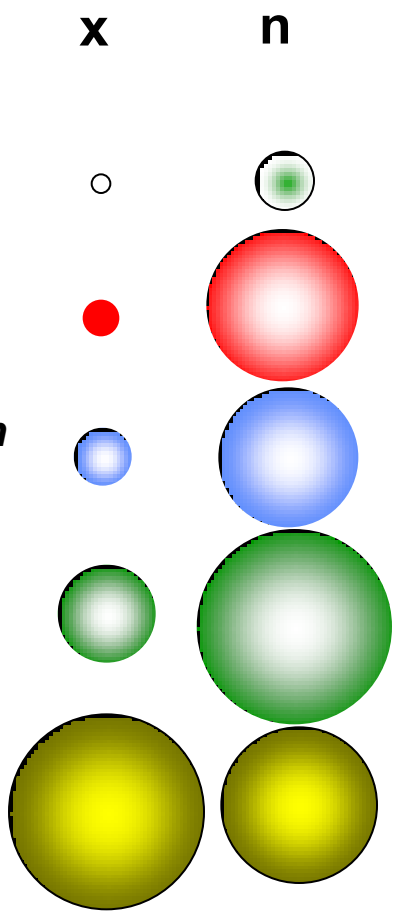
Atomic Number

Scattering Lengths :

Comparison on Neutron & X-Ray Scattering by Various Elements

Element	Neutrons (10^{-12} cm)	X-rays (10^{-12} cm)	Electrons (Z^2)
^{1}H	-0.374	0.28	1
^{2}H (D)	0.667	0.28	1
C	0.665	1.67	6
N	0.940	1.97	7
O	0.580	2.25	8
P	0.520	4.23	15

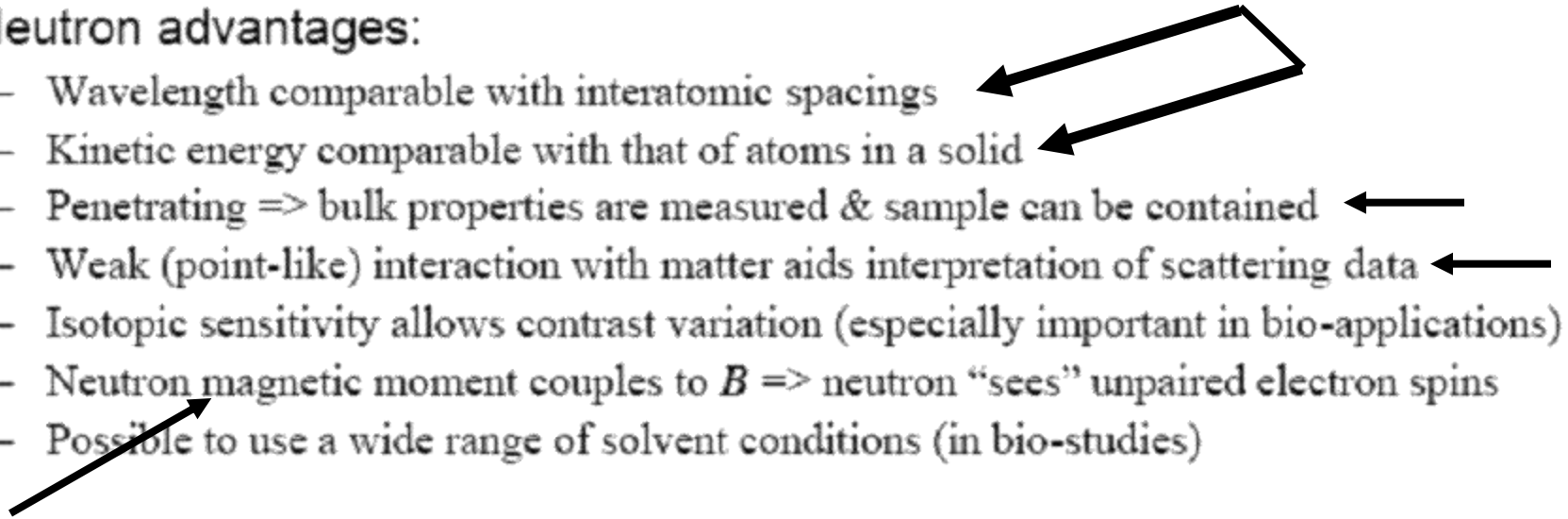
Hydrogen Isotopes are the most useful



Scattering length is like index of refraction in optics

Neutrons: Why and why not ?

- Neutron advantages:
  - Wavelength comparable with interatomic spacings
  - Kinetic energy comparable with that of atoms in a solid
  - Penetrating => bulk properties are measured & sample can be contained
  - Weak (point-like) interaction with matter aids interpretation of scattering data
  - Isotopic sensitivity allows contrast variation (especially important in bio-applications)
  - Neutron magnetic moment couples to B => neutron "sees" unpaired electron spins
  - Possible to use a wide range of solvent conditions (in bio-studies)



- Neutron Disadvantages
  - Neutron sources are weak => low signals, need for large samples etc
  - Neutrons are only available at centralized facilities & are expensive
  - Some elements (e.g. Cd, B, Gd) absorb strongly
  - Kinematic restrictions (can't access all energy & momentum transfers)
  - Measured data needs to be corrected for "instrumental effects"
  - The measured signal may correspond to a combination of physical phenomena

Outline

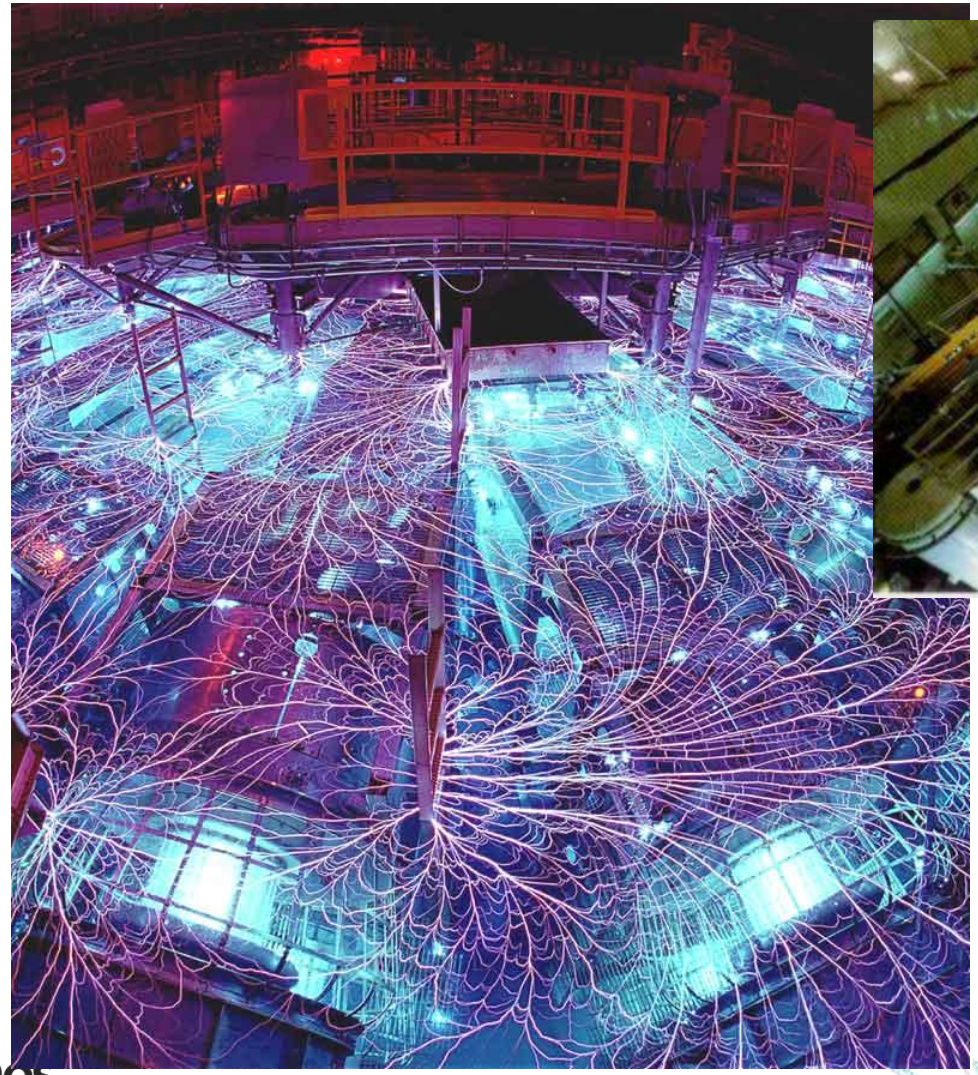
- Making neutrons
- Using neutrons and why
- **User Facilities**
- Success stories

The real base of science is those big labs

--European physicist at ILL on the NNSA labs

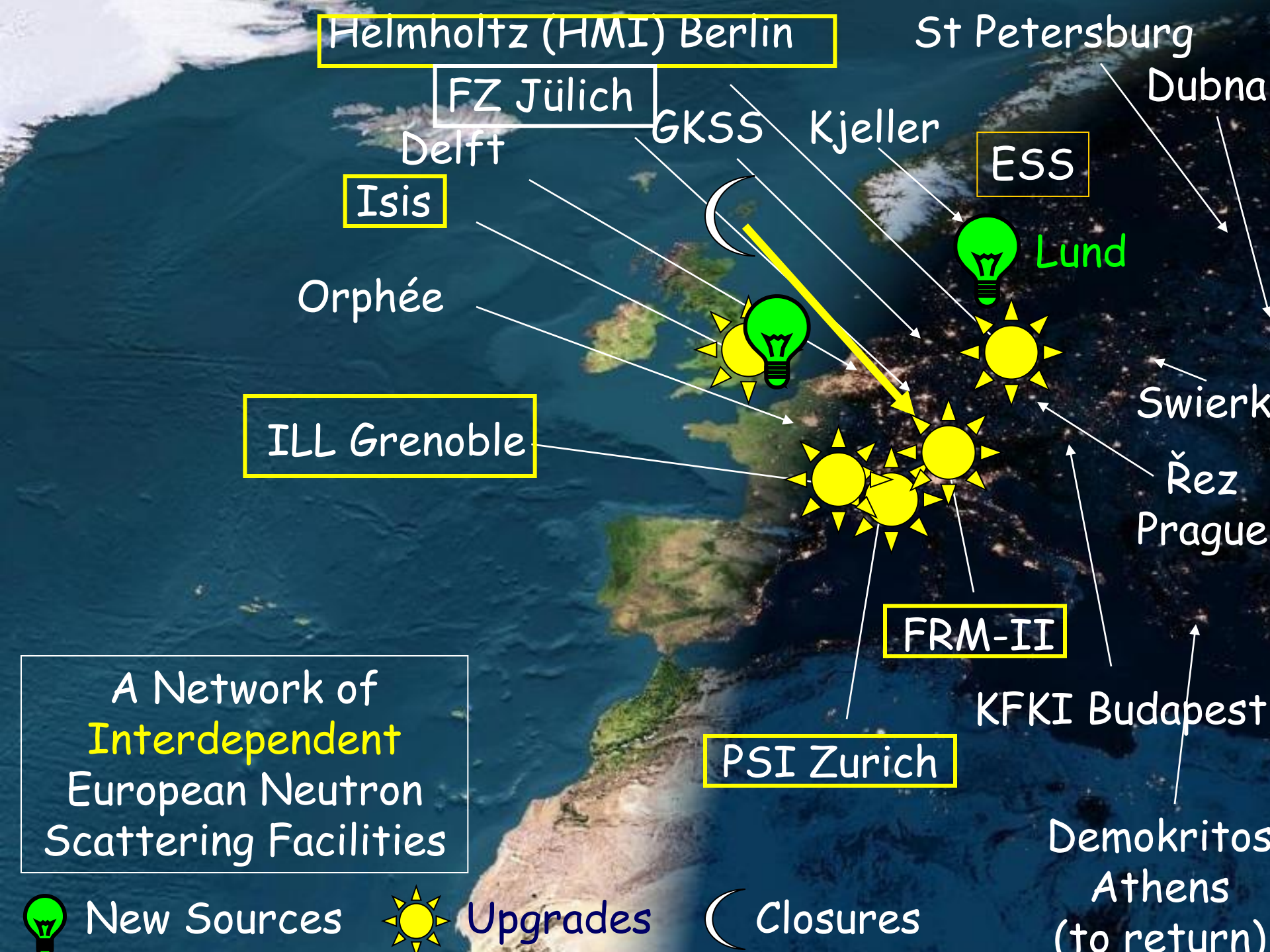
Livermore: NIF

Sandia: Z

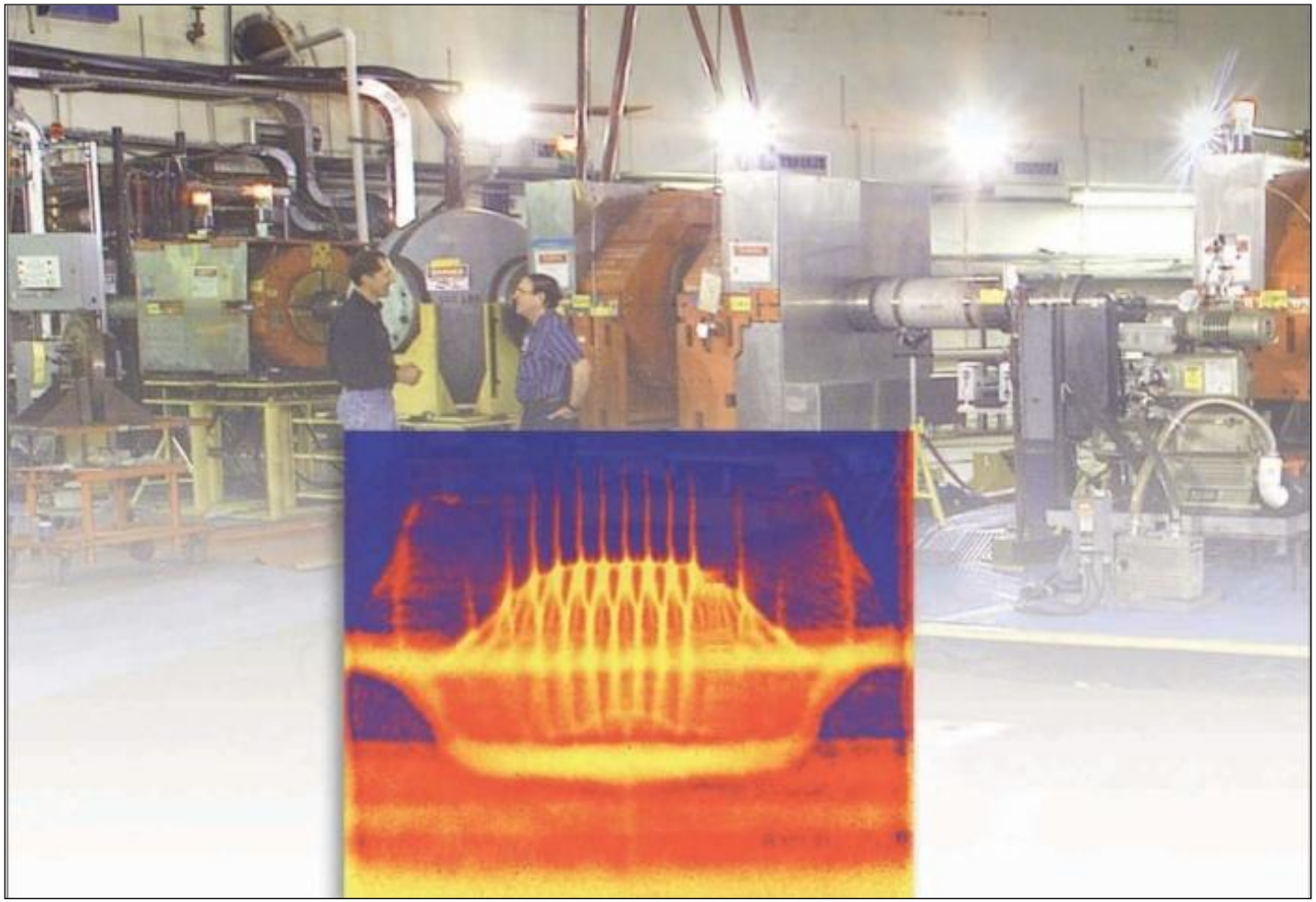


LANSCE Serves Multiple Facilities for Basic and Applied Research

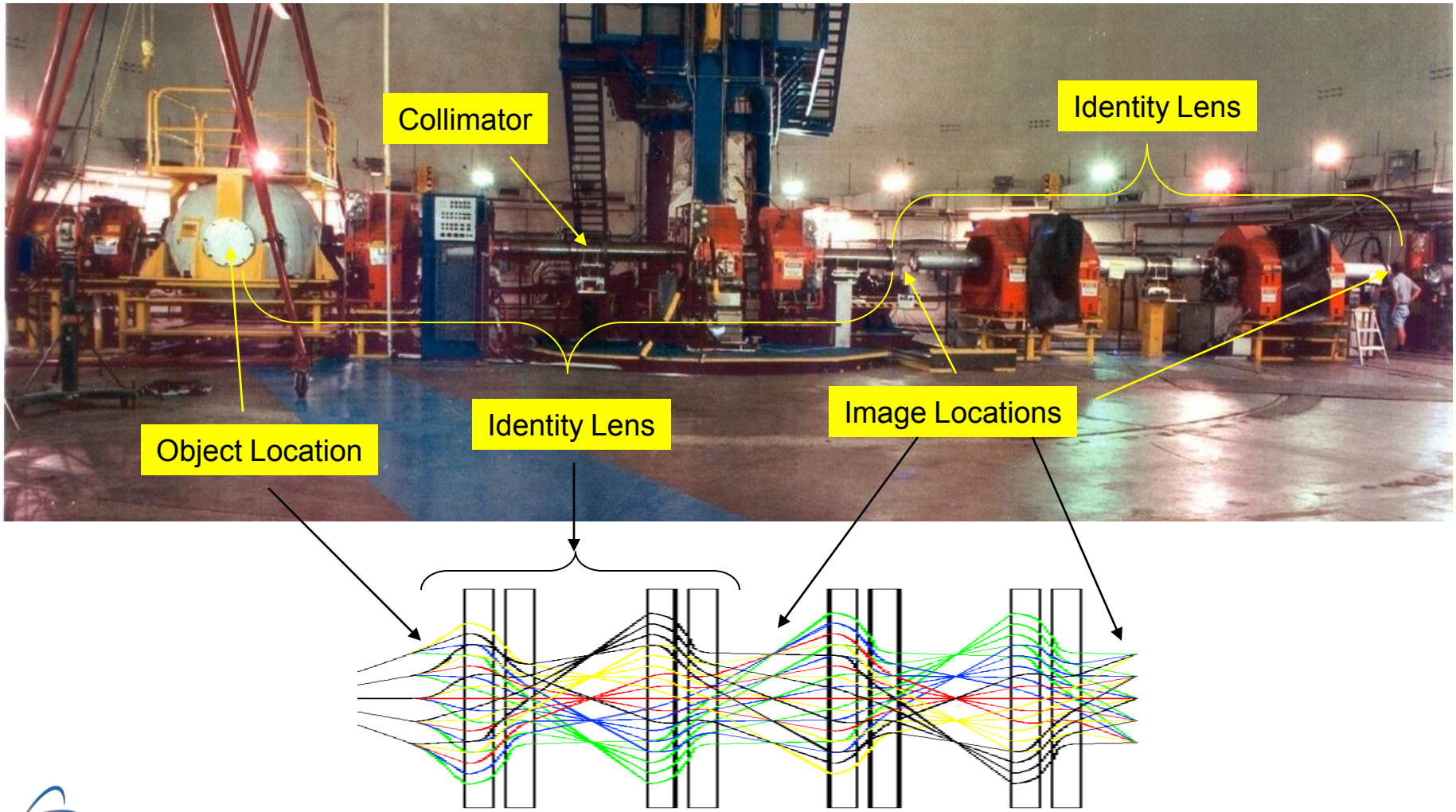
- **Lujan Center**
  - *Materials, condensed-matter, bio and nuclear physics*
  - *A BES national user facility for neutron scattering*
- **WNR**
  - *Nuclear Physics*
  - *Neutron Irradiation*
  - *SIU electronics testing*
- **Proton Radiography**
  - *Dynamic Materials science, HE science*
  - *Shock physics and Hydrodynamics*
- **Isotope Production Facility**
  - *Medical radioisotopes*
  - *Research radioisotopes*
- **Materials Test Station**
  - *Fission-Fusion-Materials Facility*
- **Ultracold Neutron Facility**
  - *Studies of fundamental properties of neutron*


Helmholtz (HMI) Berlin
St Petersburg
Dubna
FZ Jülich
GKSS
Kjeller
Delft
ESS
Isis
Lund
Orphée
Swierk
ILL Grenoble
Řez
Prague
FRM-II
KFKI Budapest
PSI Zurich
Demokritos
Athens
(to return)
A Network of
Interdependent
European Neutron
Scattering Facilities
New Sources
Upgrades
Closures

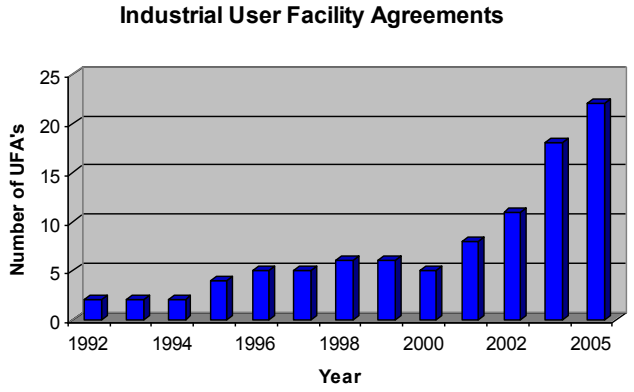
Proton Radiography reveals dynamics of matter at microsecond scale



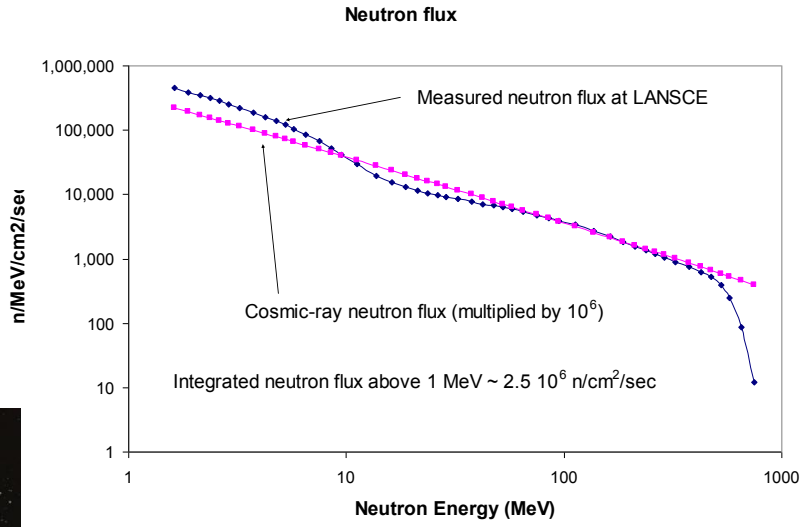
pRad Facility at LANSCE



LANSCE/WNR is a unique national resource for single-event-upset testing of critical components



WNR offers a neutron spectrum similar to that of cosmic rays

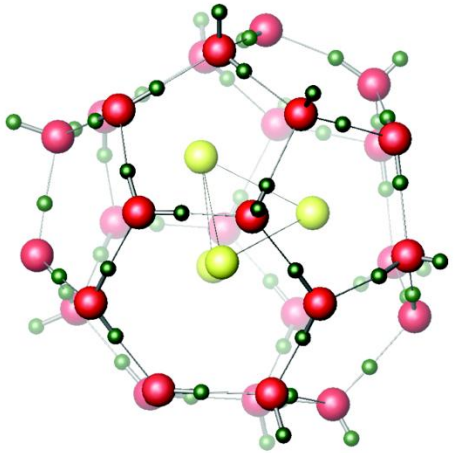


Reliable Satellites

Safer Avionics

Server Surety

The Lujan Center neutrons play a key role in research for energy and the environment.

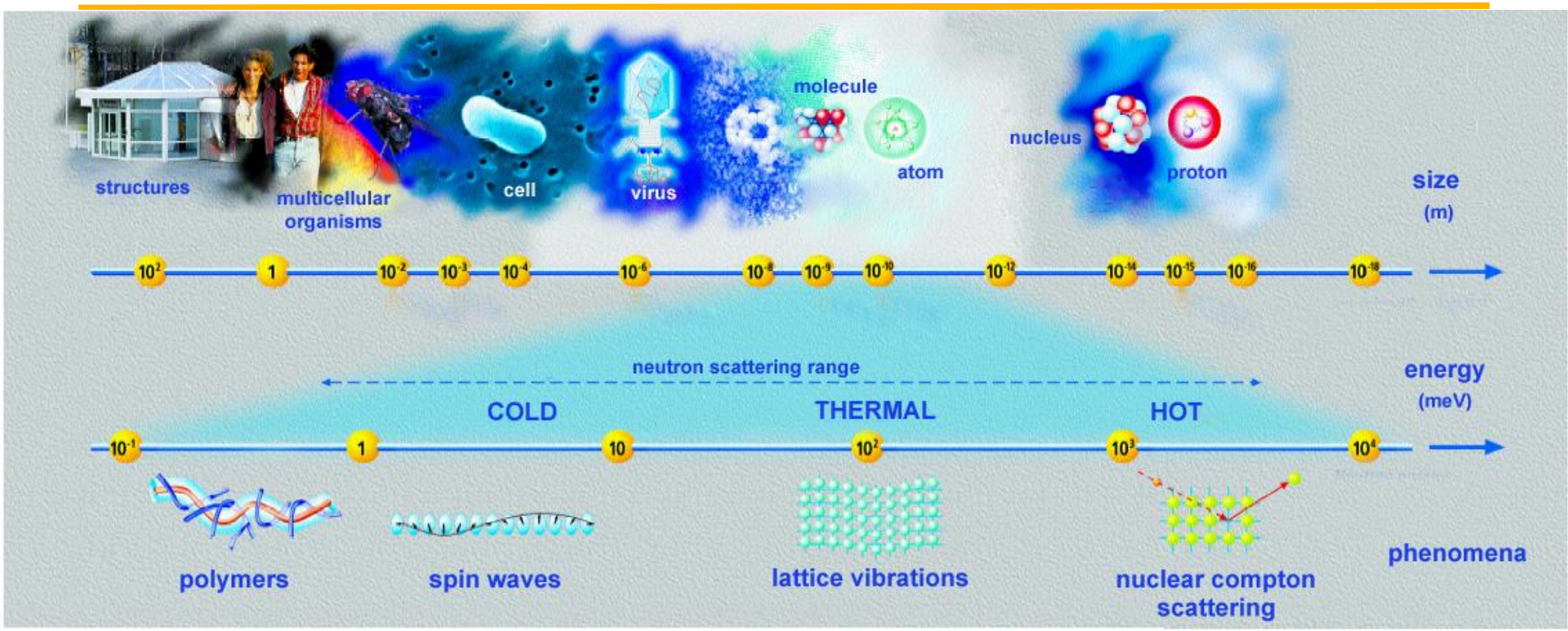


Hydrogen storage, biofuels, and complex electronic materials

Hard materials

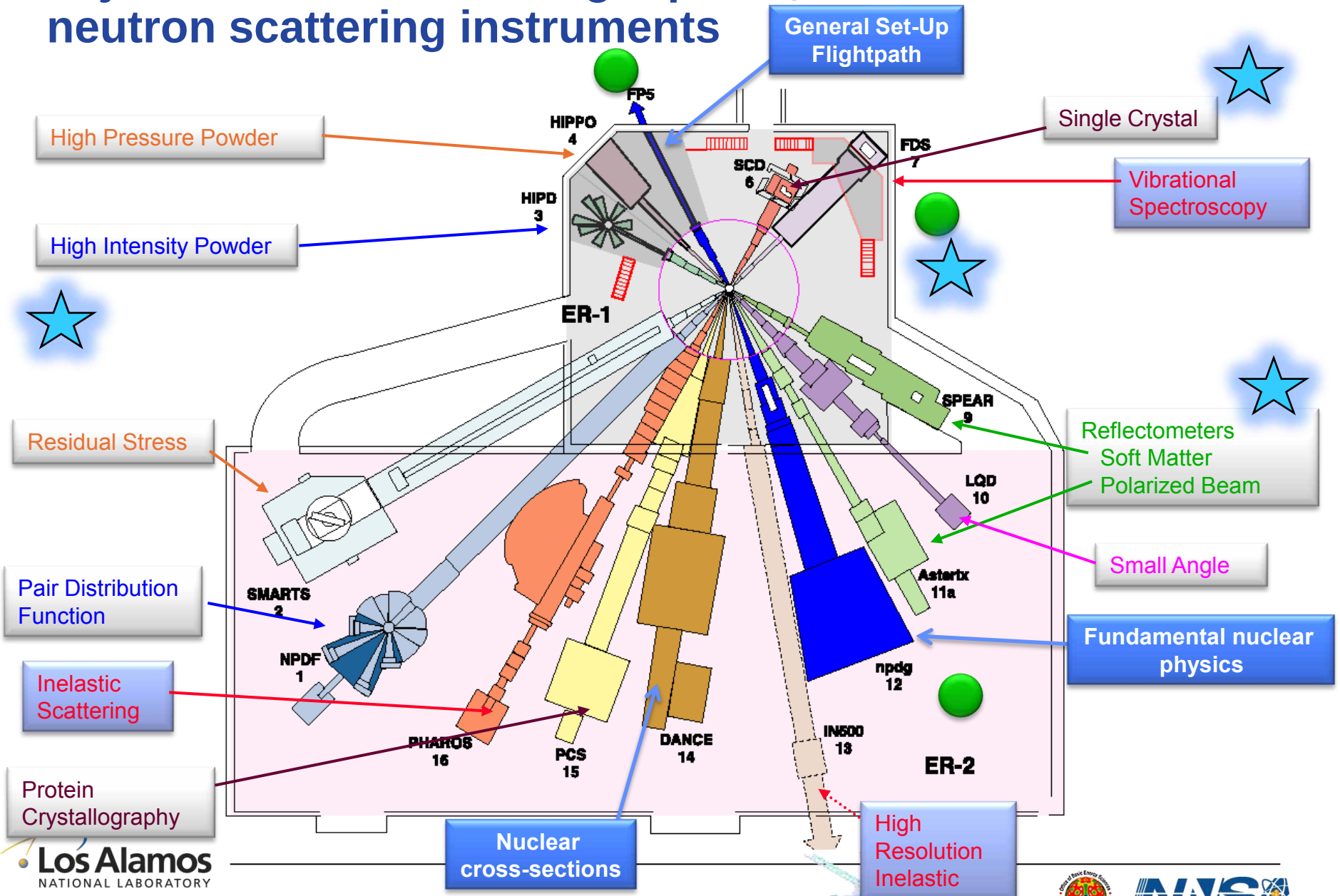
Nuclear fuel cycle

Neutron scattering has advantages in studies of many energy materials-related phenomena



Sensitivity to hydrogen and other light elements
Isotopic distinctions
Magnetism
Penetrability even in heavy metals

Lujan Center 2010: 16 flight paths, 11 of which have neutron scattering instruments



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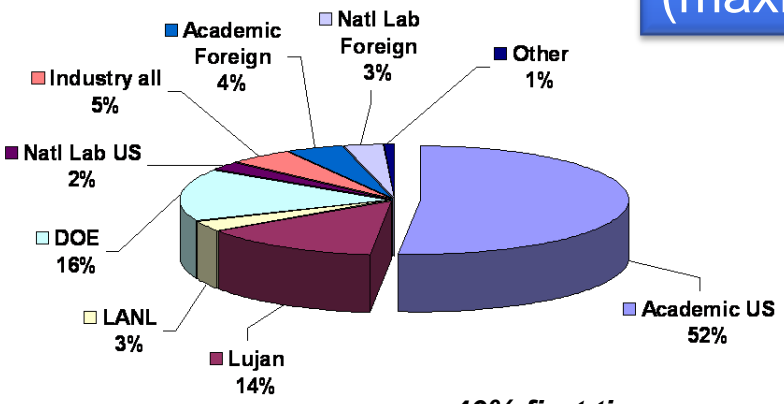
LUJAN CENTER

NNSA

The Lujan Neutron Scattering Center at LANSCE Hosts up to 750 Researchers Per Year

- National User Program
- Neutron Scattering School August 2010
- Affiliated with LANL's CINT and Magnet Lab

2010: Run 3000 hours, 126 days (maximum is 4500 hours)



40% first time users

LANSCE Neutron Scattering School brings in 30 students and 20 lecturers per year

Los Alamos NATIONAL LABORATORY EST. 1943

LANSCE Neutron School 2010: Structural Materials

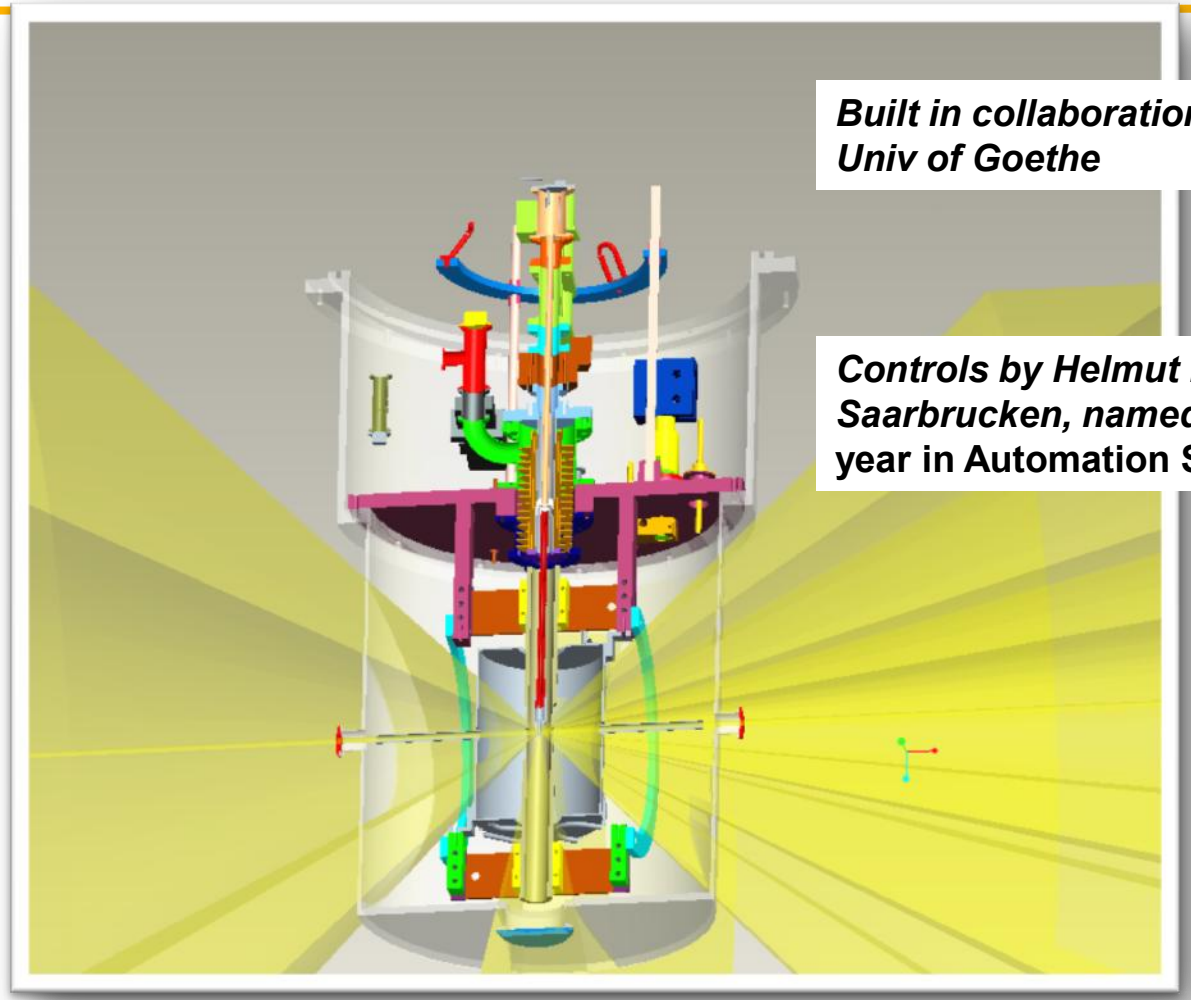
www.lansce.lanl.gov/neutronschool
dbrown@lanl.gov

Los Alamos NATIONAL LABORATORY EST. 1943

LANSCE LUJAN CENTER Los Alamos National Laboratory

NNSA

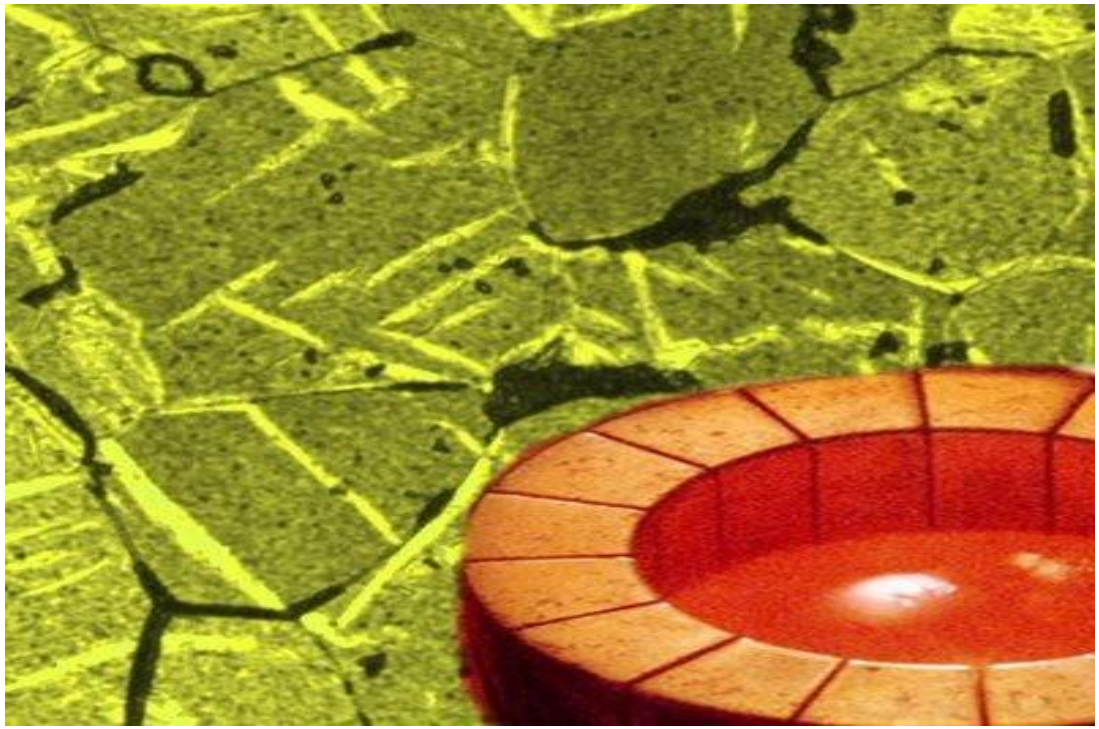
The new HIPPO graphite furnace has achieved 2200C, designed for 3000C



Built in collaboration with Bjorn Winkler, Univ of Goethe

***Controls by Helmut Reiche, HTW Saarbrucken, named "*best student of the year in Automation Systems"**

Actinide-science problems are familiar materials challenges: Structure-Property Relations



Plutonium science

Multiphase Equations of State

Most electronic theories of Pu predict magnetism

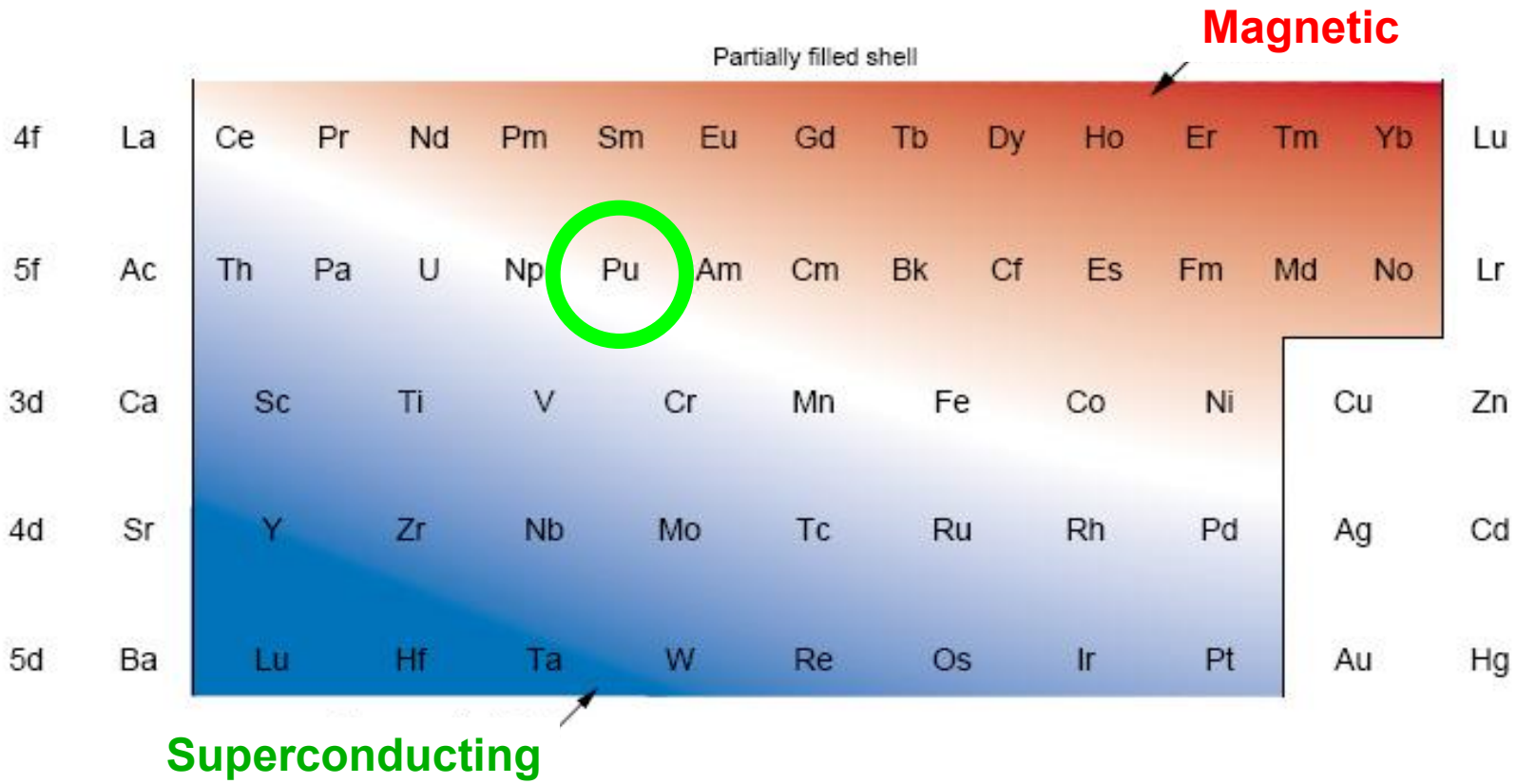
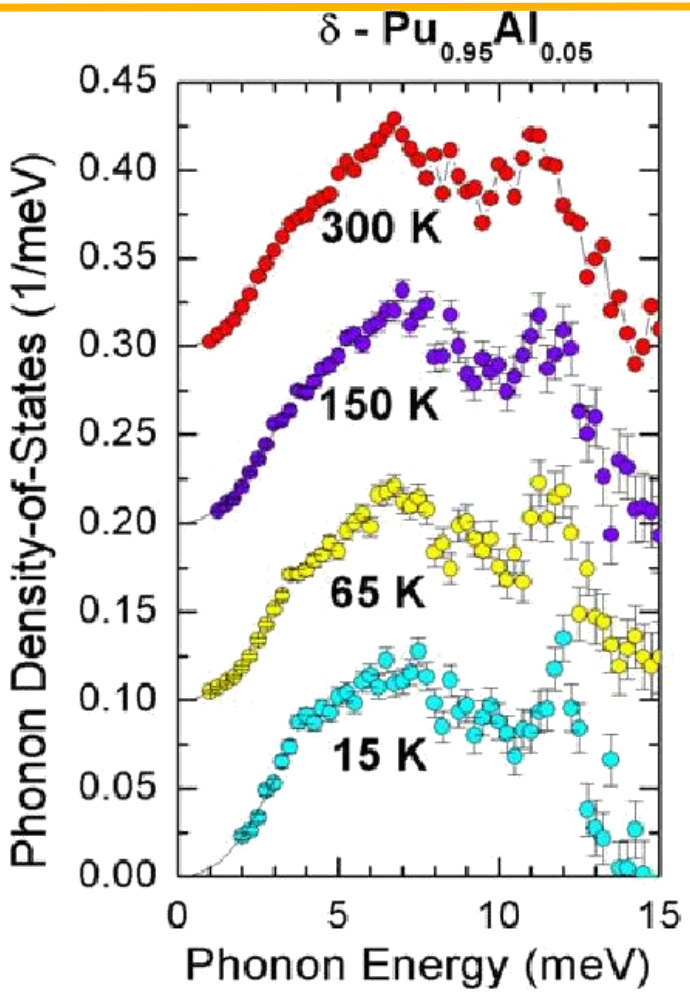


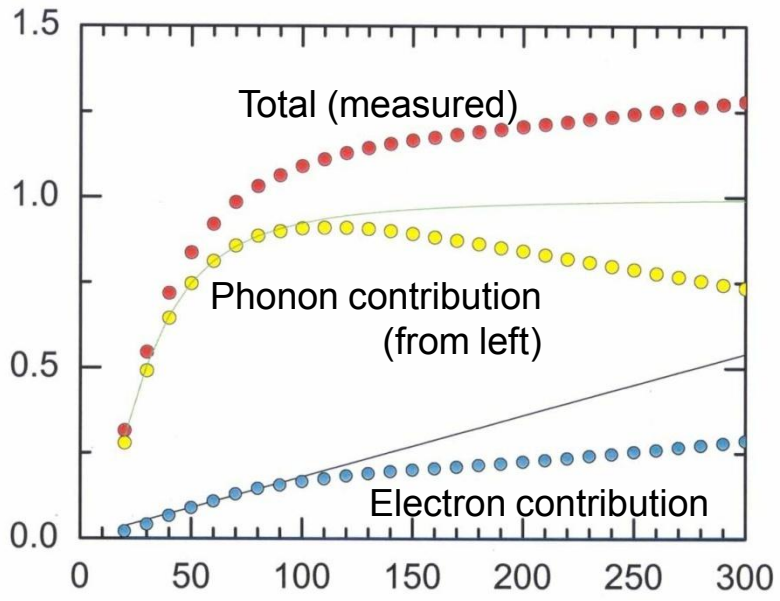
Figure 19. A Revised Periodic Table of the f and d Series

Logic: Large volume expansion from a to d
Implies: Five of six 5f electrons are localized
Implies: An unpaired electron
Requiring: Large magnetic moment

Inelastic neutron scattering on Pharos gave first look at phonon and electron contributions to Pu thermodynamics.



Specific Heat

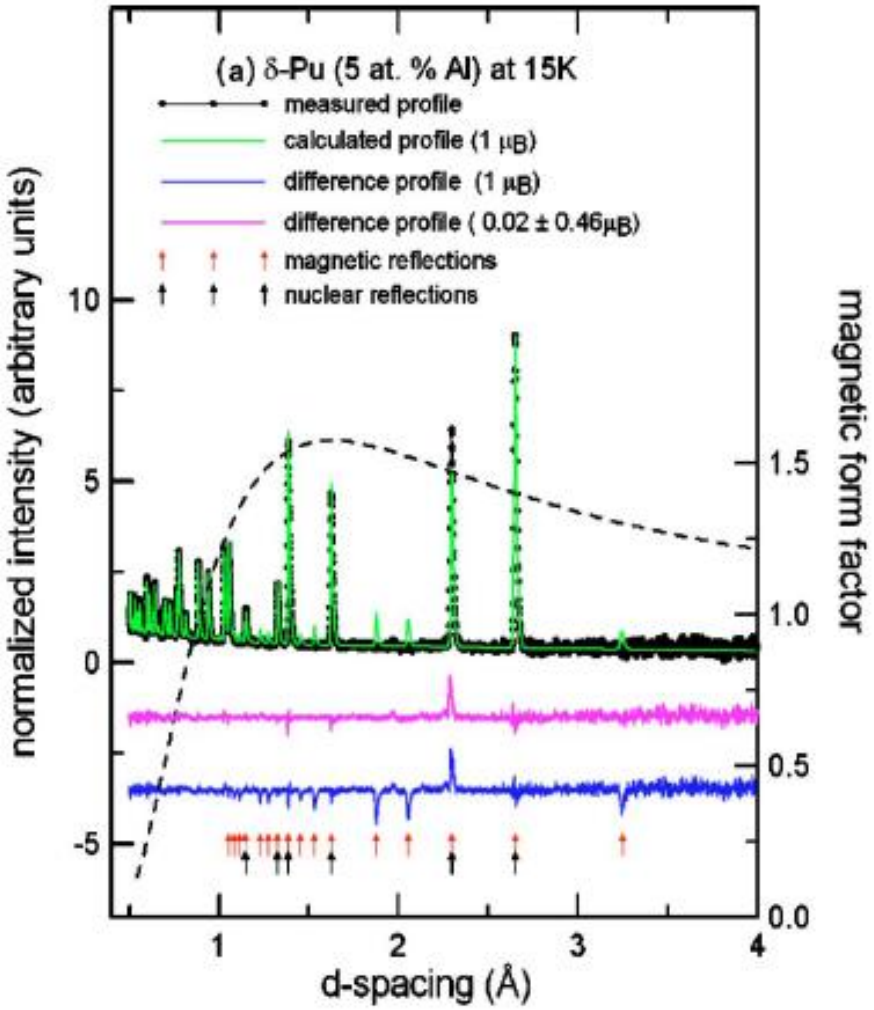


McQueeney et al, PRL 2003

PHYSICAL REVIEW B 72, 054416 (2005)

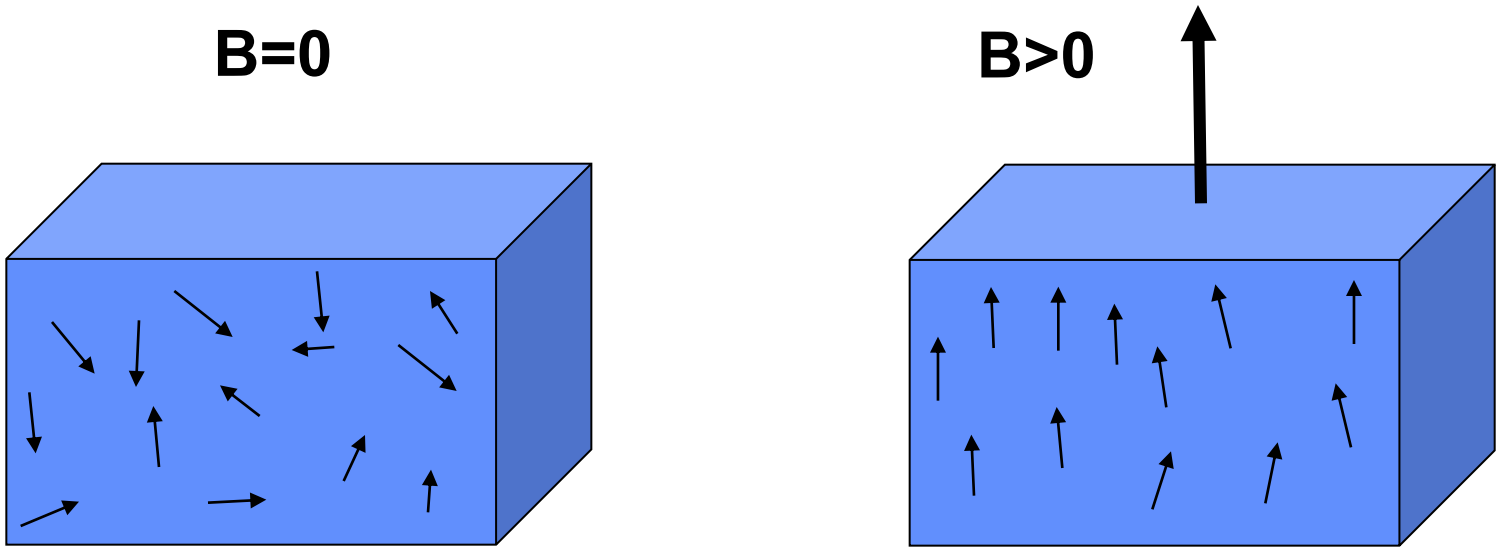
Absence of magnetic moments in plutonium

J. C. Lashley,[1] A. Lawson,[1] R. J. McQueeney,[2] and G. H. Lander[3]
[1]*Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[2]*Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA*
[3]*European Commission, JRC, Institute for Transuranium Elements, Postfach 2340, Karlsruhe, Germany*
(Received 25 June 2004; revised manuscript received 29 November 2004; published 11 August 2005)



HIPD 2005

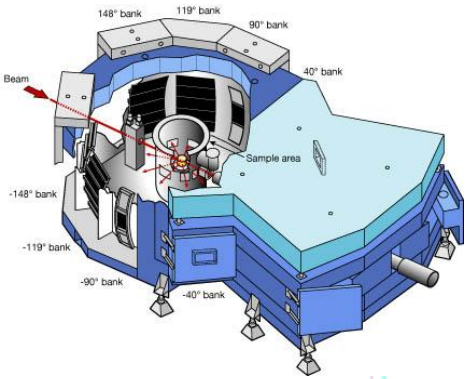
A magnetic field might align the localized moments…

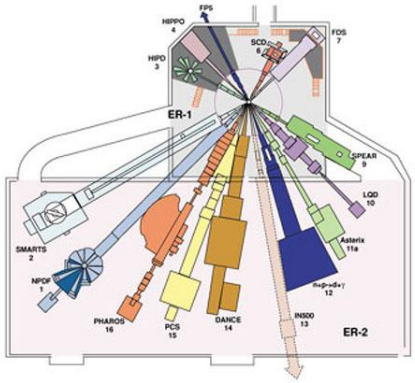


PDF Group at the Lujan Center

We are using and developing total scattering methods to characterize disordered crystalline, nano- and amorphous materials.

- **Facilities**
  - Lujan Center
  - Advanced Photon Source
  - "One-stop" proposal for both facilities
  - Complementary data on local structure





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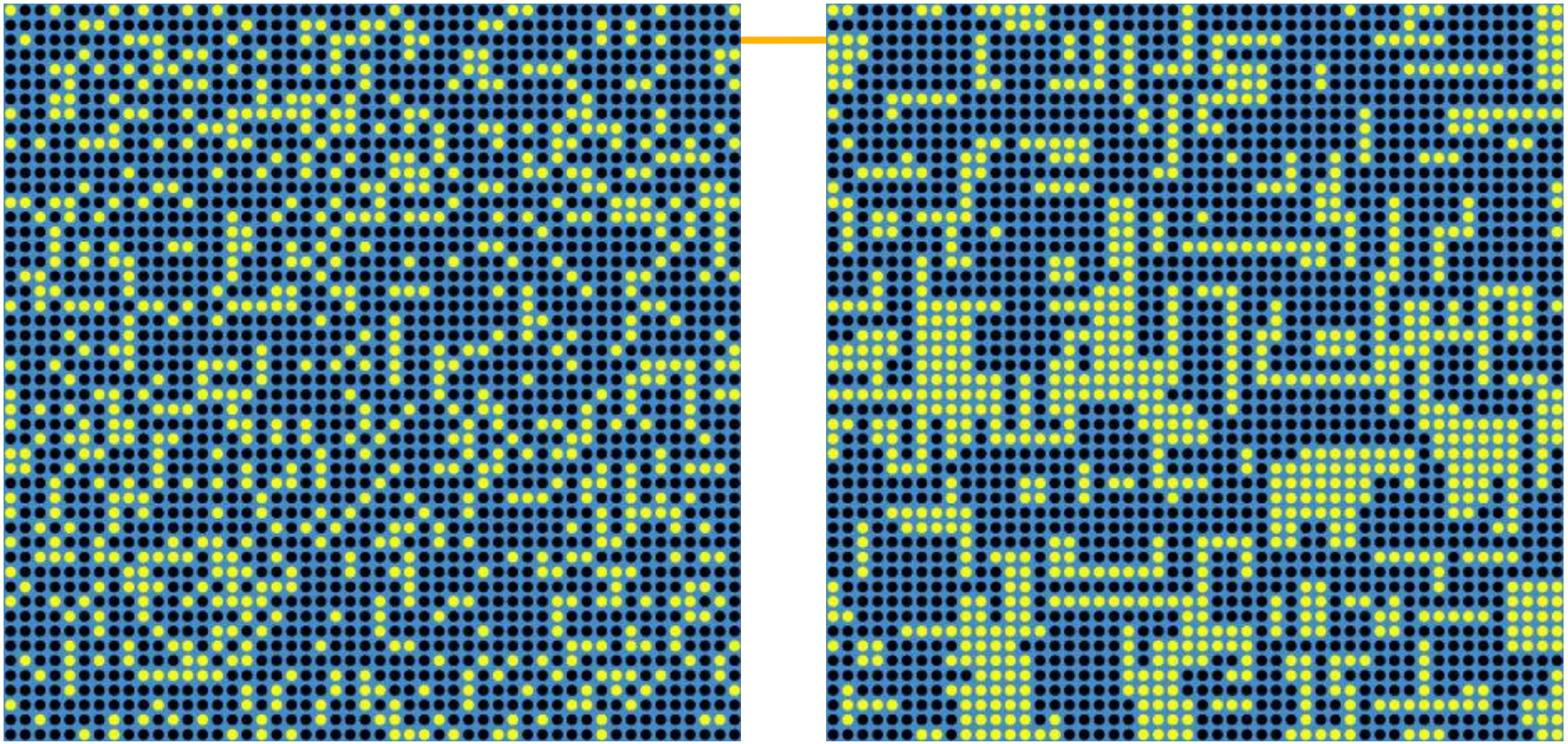
LUJAN CENTER

NNSA

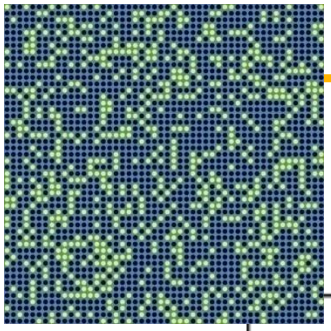
Disordered materials
(acknowledgment: Thomas Proffen)



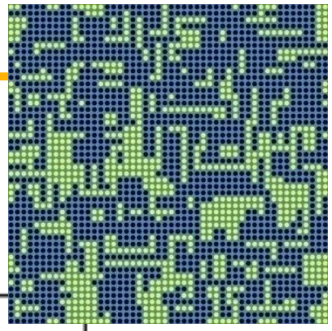
Cross section of 50x50x50 u.c. model crystal consisting of 70% black atoms and 30% *vacancies* !

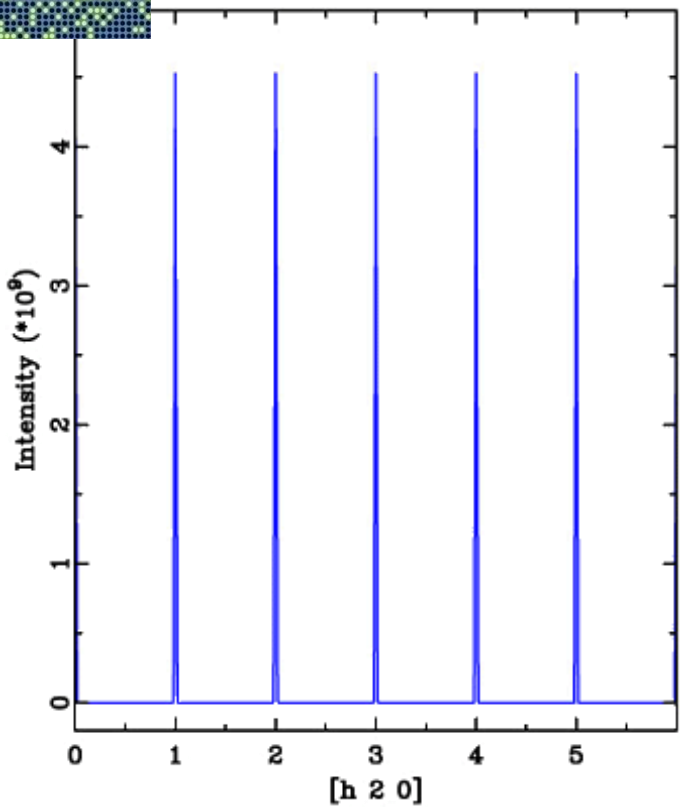
Properties might depend on vacancy ordering !!

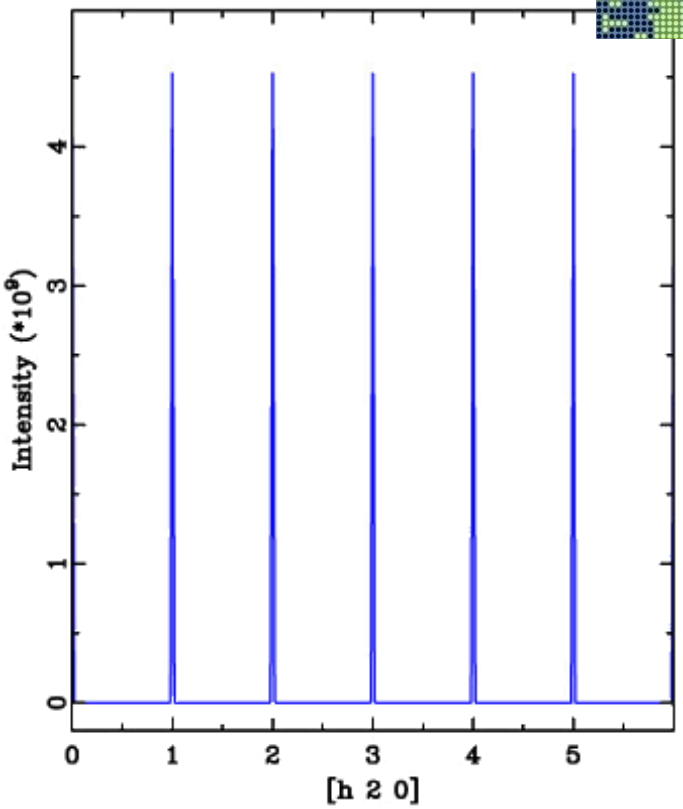
Bragg peaks are blind to local structure



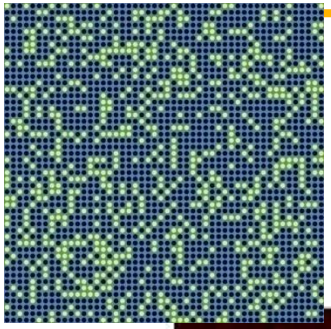
Bragg scattering: Information about the *average* structure, *e.g.* average positions, displacement parameters and occupancies.



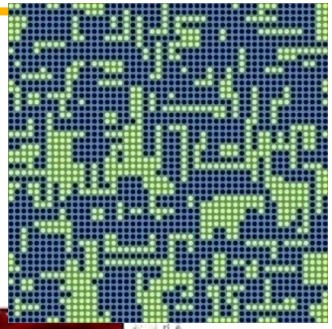


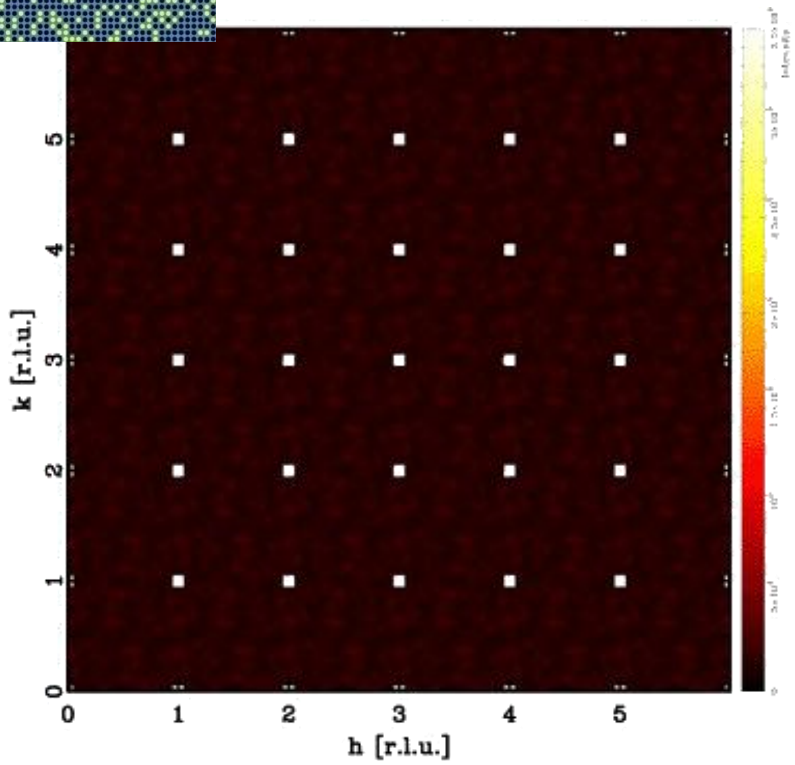


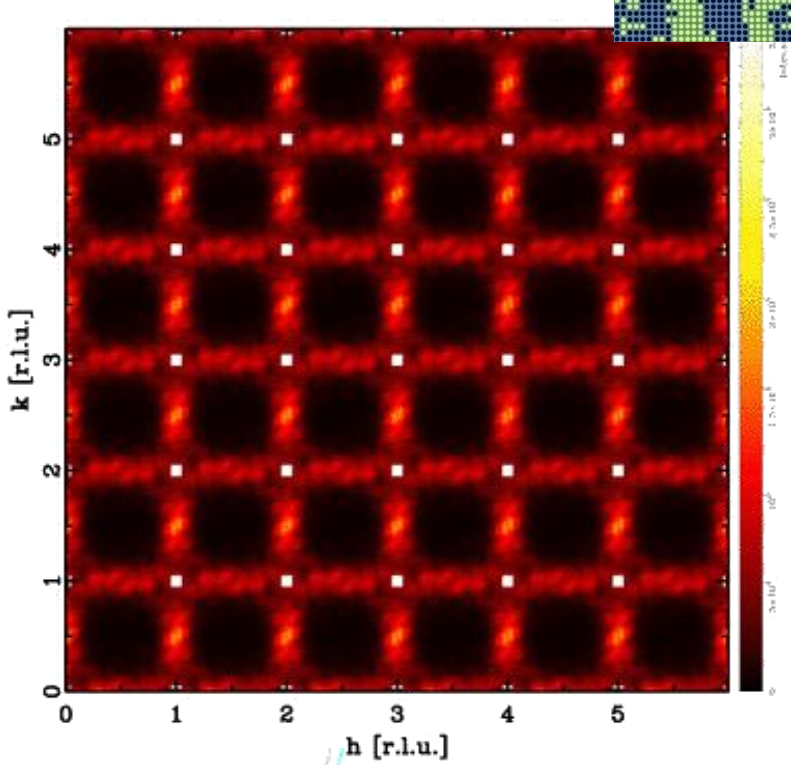
Diffuse scattering encodes correlations



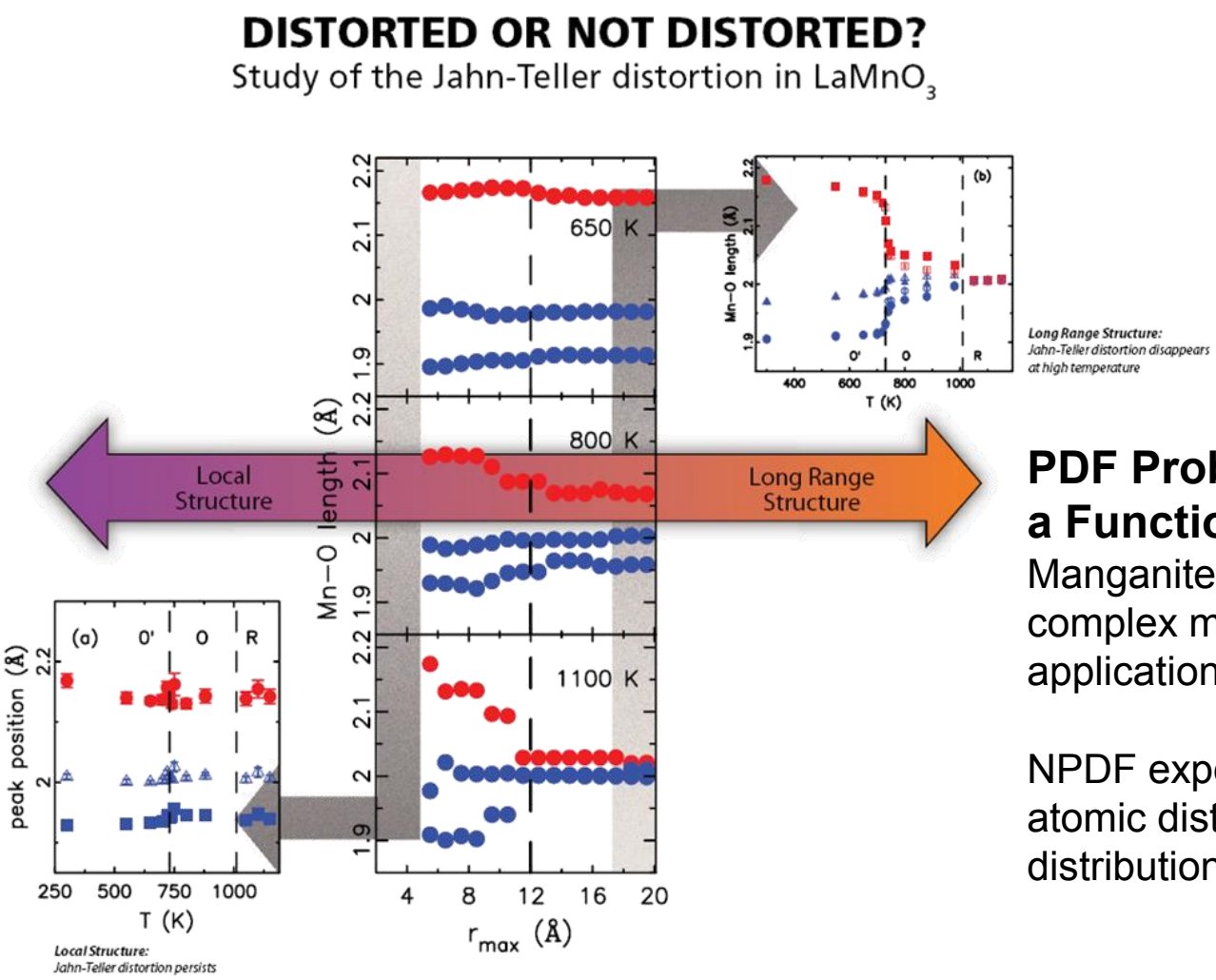
Diffuse scattering: Information about *two-body correlations*, *i.e.* chemical short-range order or local distortions.







NPDF unravels the local structure in $LaMnO_3$



NPDF

Instrument Scientist

Thomas Proffen

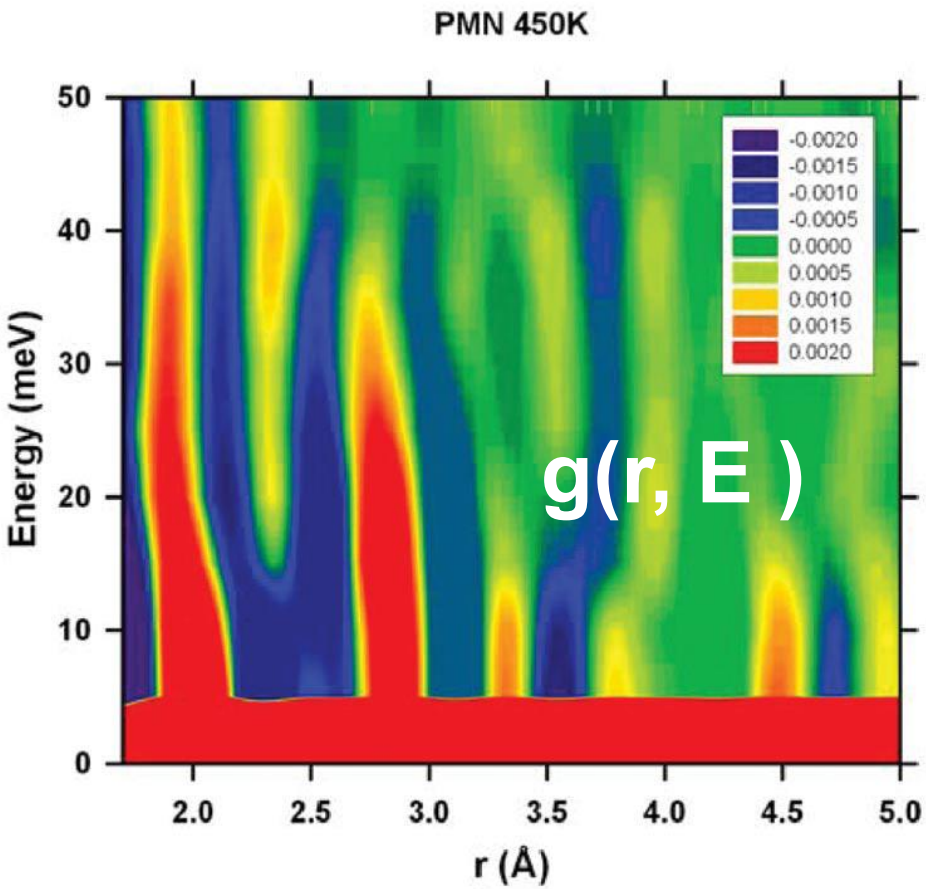
PDF Probes the Structure as a Function of Length Scale

Manganites are among the many complex materials used in energy applications all around us.

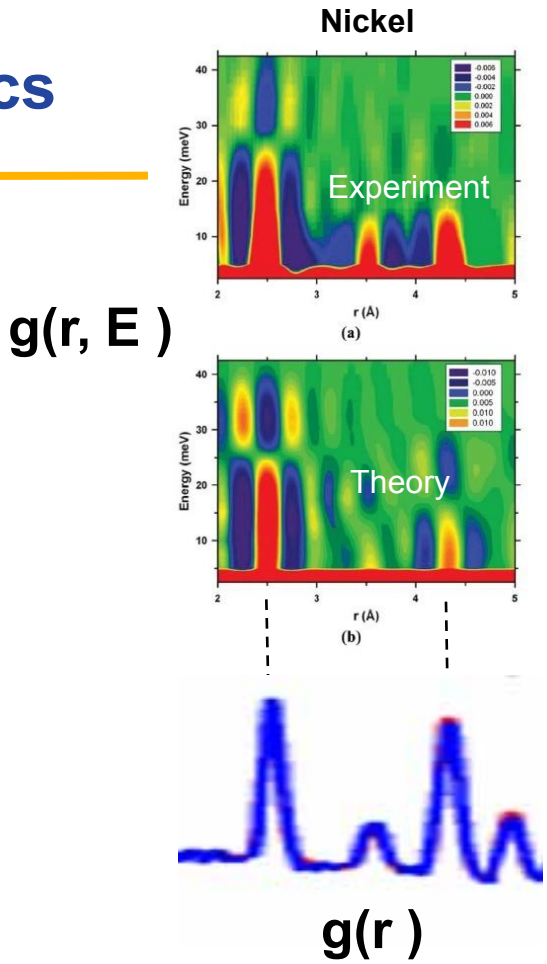
NPDF experiments revealed local atomic distortions and their distribution

X. Qiu, Th. Proffen, J.F. Mitchell and S.J.L. Billinge, **Orbital correlations in the pseudo-cubic O and rhombohedral R phases of LaMnO3**, *Phys. Rev. Lett.* **94**, 177203 (2005).

Dynamic Pair Distribution Function analysis demonstrated on ferroelectrics



Relaxor Ferroelectric PMN has local regions of electric polarity due to Pb-O distance changes caused by phonons



Led by Takeshi Egami, Univ of Tennessee
PRL **100, 137602 (2008)**

Los Alamos NATIONAL LABORATORY EST. 1943

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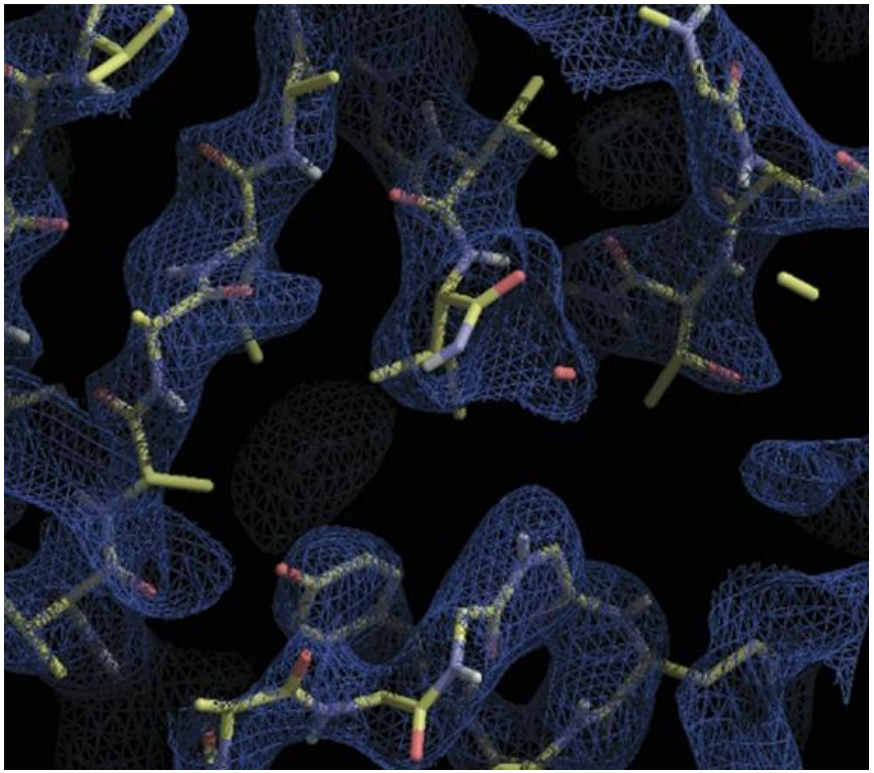
NNSA

Neutron scattering at PCS* is a powerful tool in bioscience research.

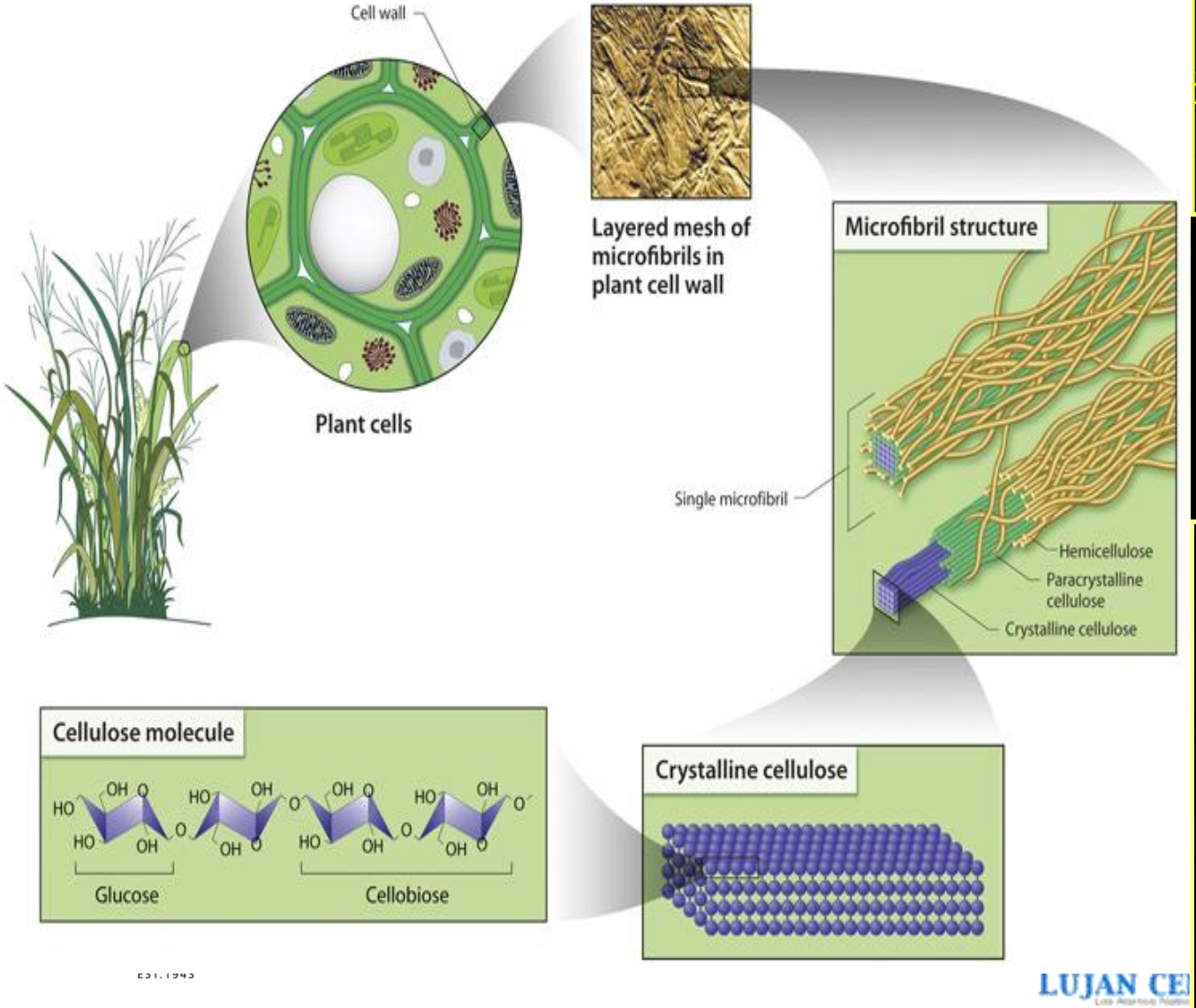


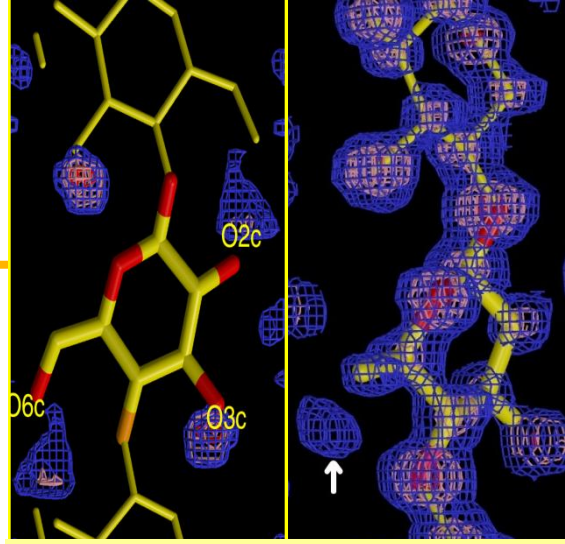
- Can reveal structural details, such as the locations of hydrogen atoms and water molecules
- Pinpoints biochemical steps involved in enzyme reactions
- Improves understanding of cellular processes
- Has potential to enable design of more effective drugs for treating disease

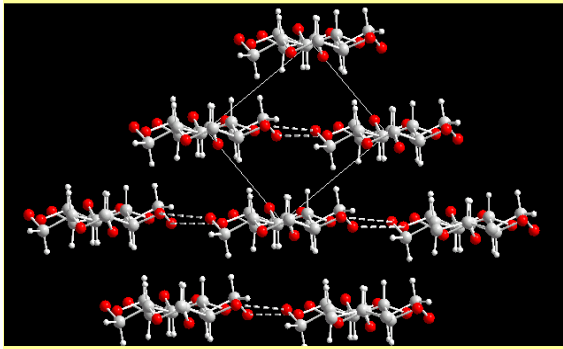
*Protein Crystallography Station

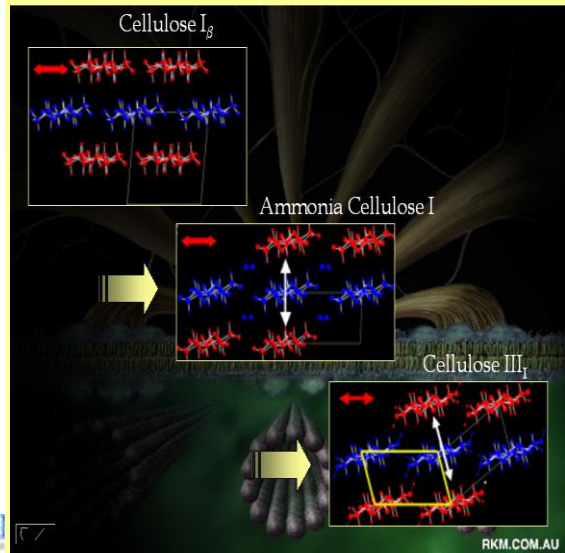
Biomass structure and conversion

For 3rd generation biofuels







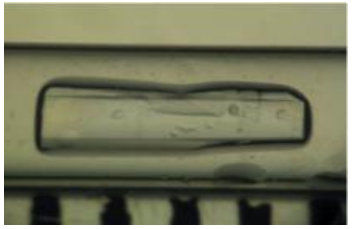


Environment and Carbon Management

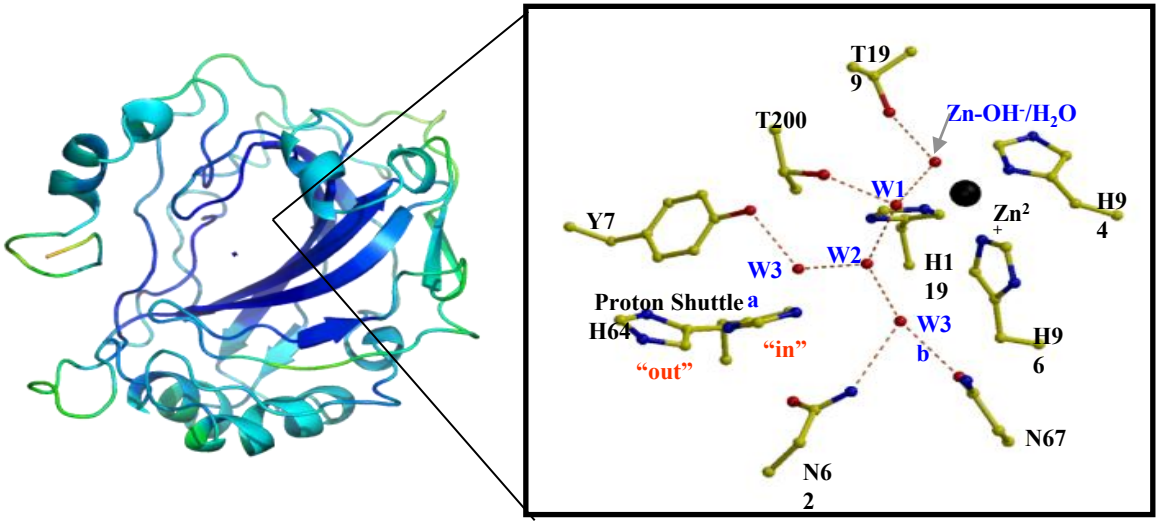
Carbonic anhydrase (CA) catalyzes the reversible interconversion of CO_2 to HCO_3^-

Understanding how the enzyme facilitates CO_2 hydration and proton transfer will help in devising methods for using biological systems for carbon sequestration.

Proton transfer between a Zn-bound water and internal proton shuttle is mediated by a H-bonded network of solvent molecules. X-ray structures do not provide needed acuity.



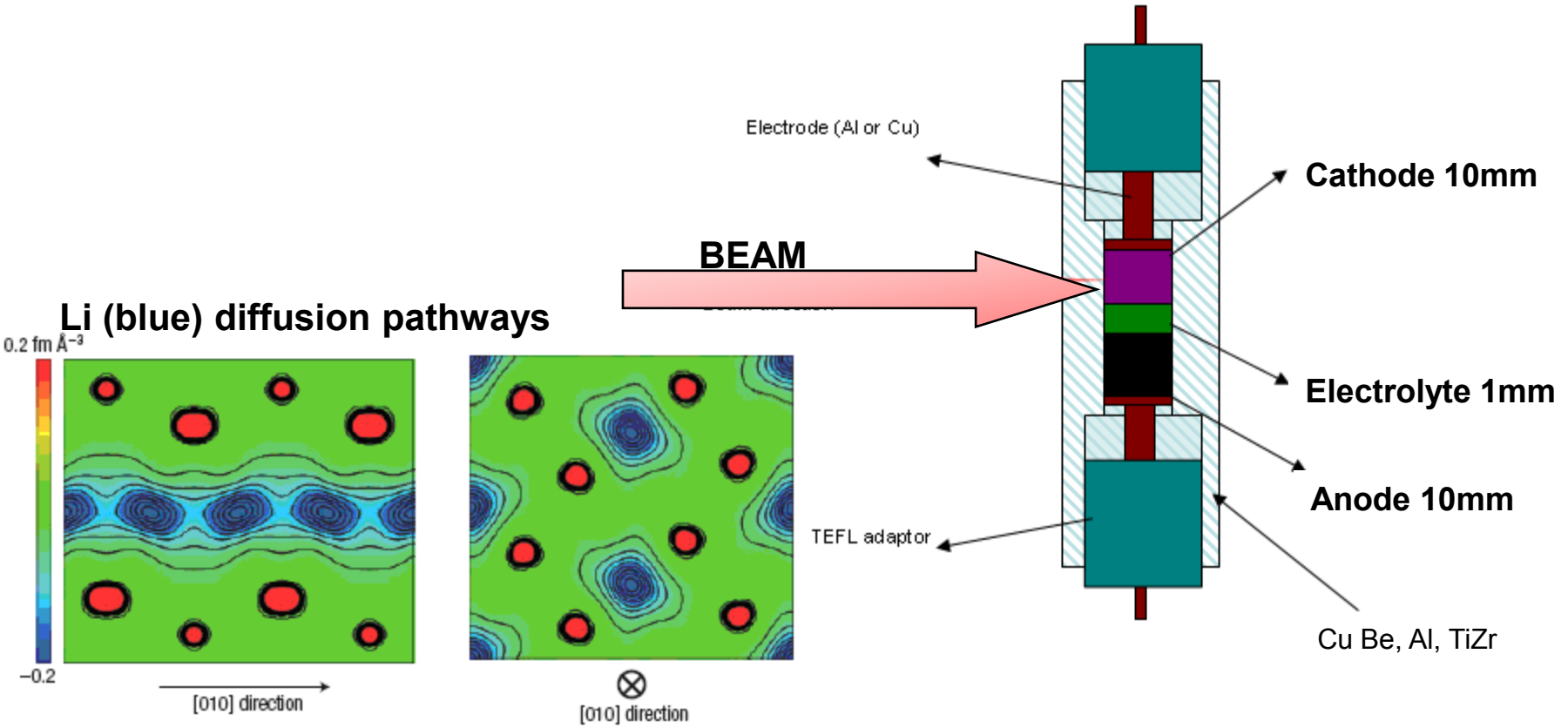
- Sample: 4 x 1 x 0.3 mm (1.3 mm^3)
- H/D exchanged for 1 month
- Collected 41 images/crystal settings
- Each exposure 32h



USERS: John Domsic, Robert McKenna, David Silverman, Zoe Fisher - University of Florida, LANL

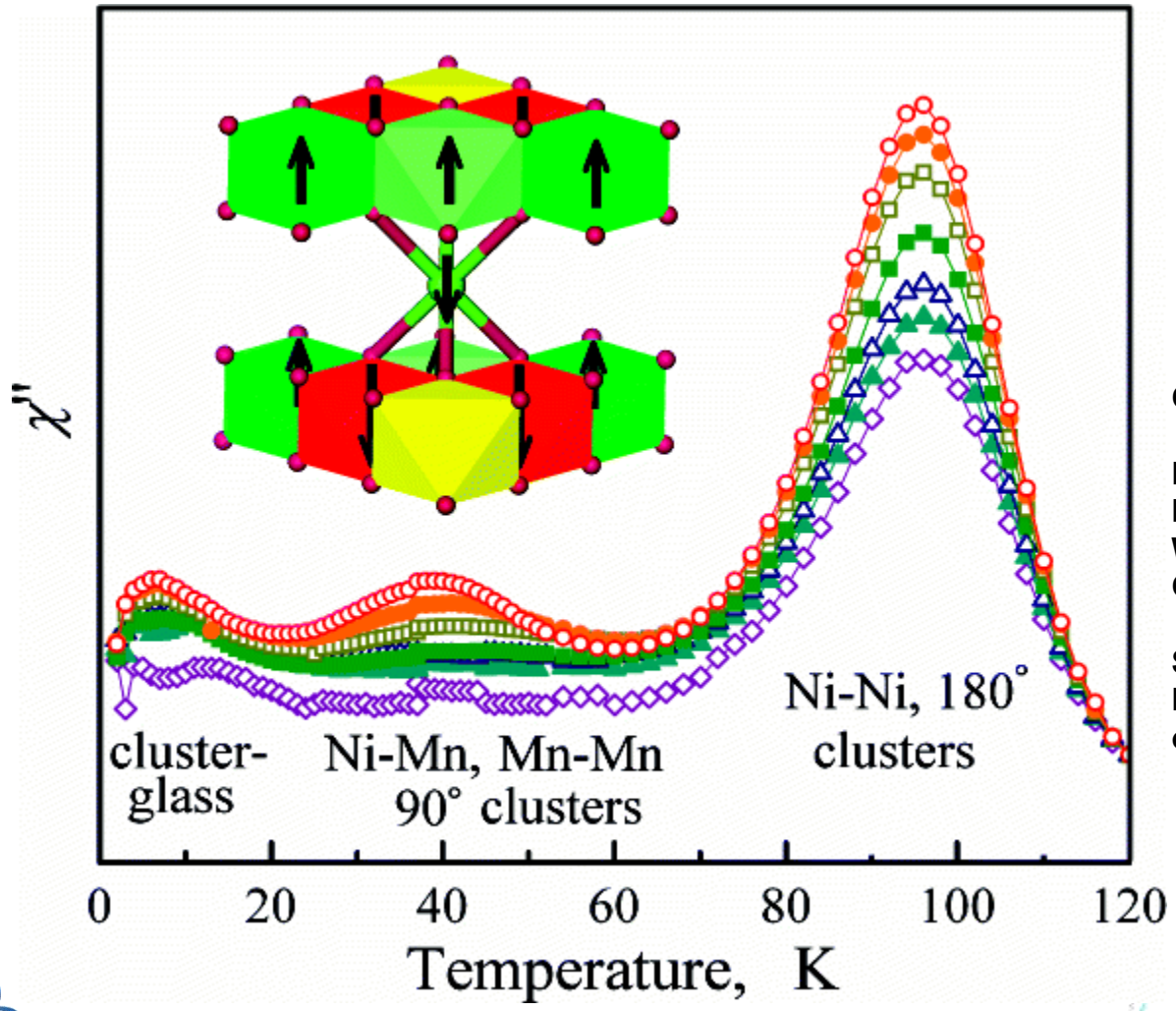
REFERENCES: Fisher *et al.* (2009) *Acta F***65**, p.495

Lujan's "standard battery cell"
Guo, Vogel, Zhao



Nishimura, et al Nature Materials, **2008, 7, 707**

Layered $Li_xNi_yMn_yCo_{1-2y}O_2$ Cathodes for Lithium Ion Batteries: Understanding Local Structure via Magnetic Properties

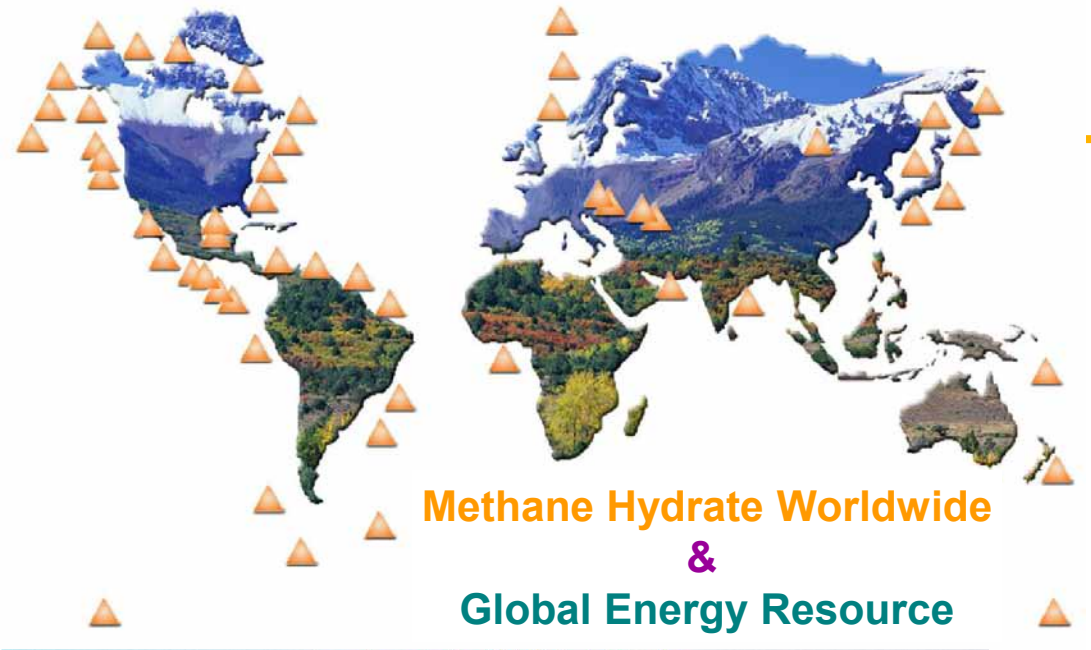


Chem of Materials 19 4682 (2007)

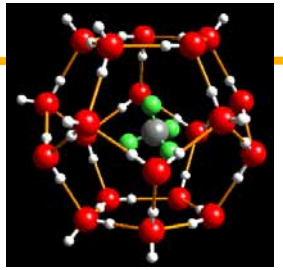
Natasha A. Chernova, Miaomiao Ma, Jie Xiao, M. Stanley Whittingham, Julien Breger, and Clare P. Grey

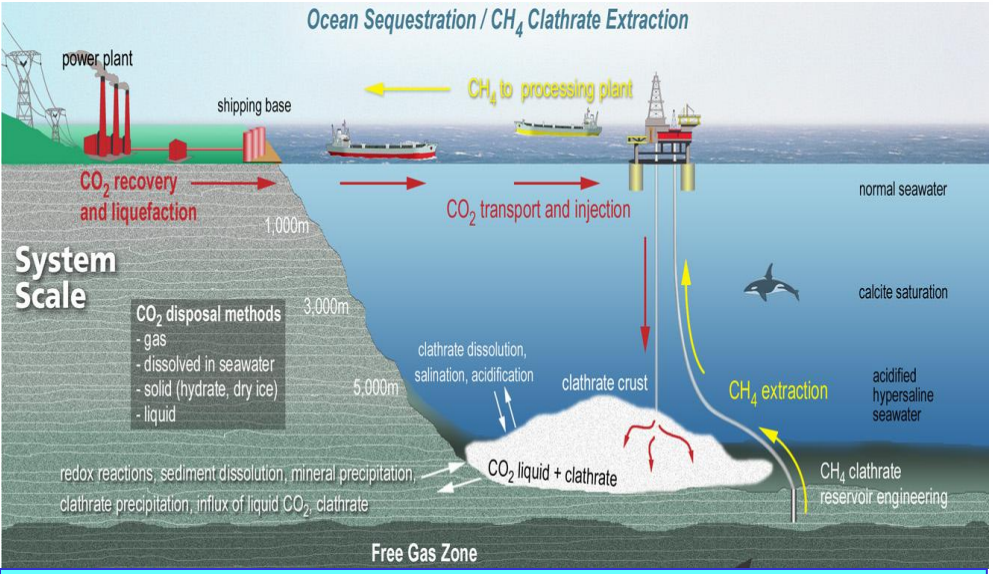
State University of New York at Binghamton, and State University of New York at Stony Brook

Grand Challenges in Geomaterials



Methane Hydrate Worldwide
&
Global Energy Resource





Global hydro-cycle and global carbon-cycle determine sustainability

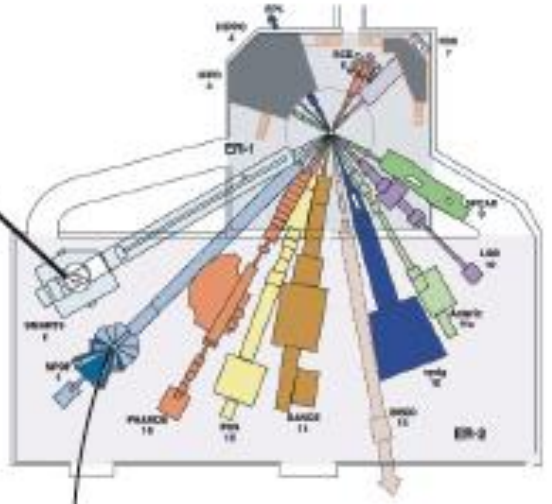
Energy CH_4 ↑ Sequestration CO_2 ↓

LUJAN CENTER

Spectrometer for Materials Research at Temperature and Stress (SMARTS)

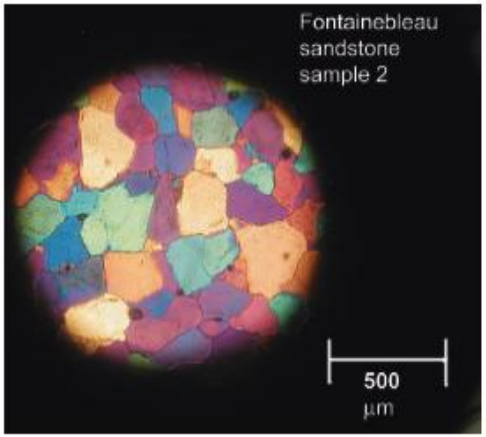
Special horizontal Instron Load Frame (left) which goes in the SMARTS "cave" at the end of the beam (right)

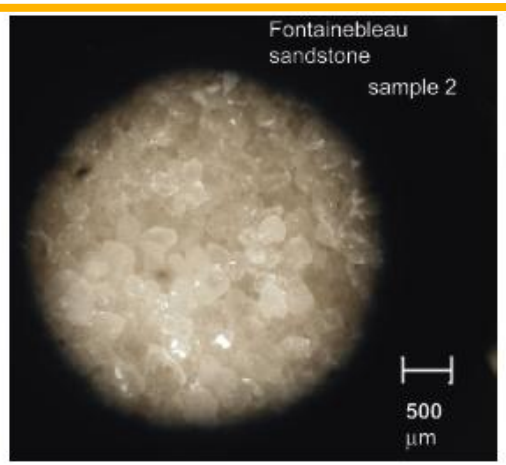
Webcam view of Fontainebleau sandstone sample in the neutron beam while stressed in the SMARTS/Instron load frame during the experiment.

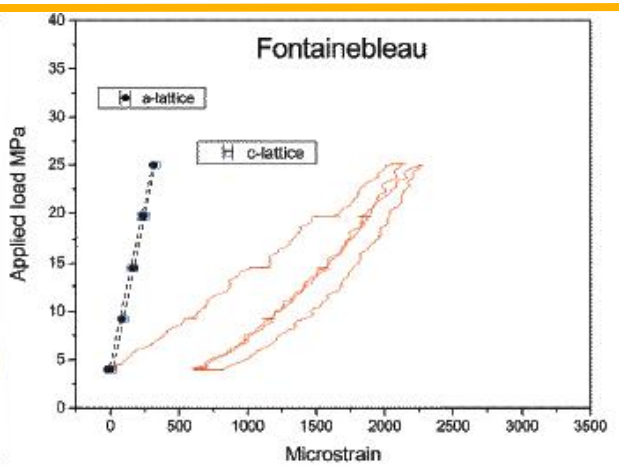


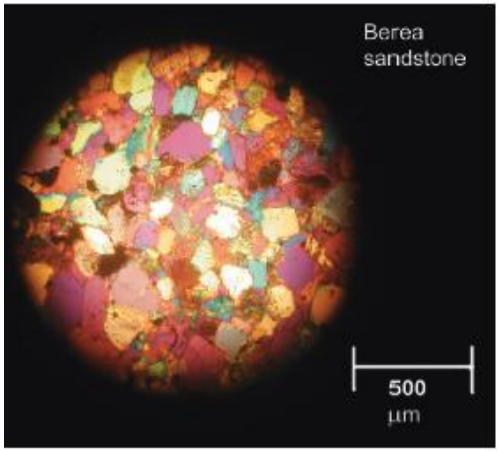
NPDF

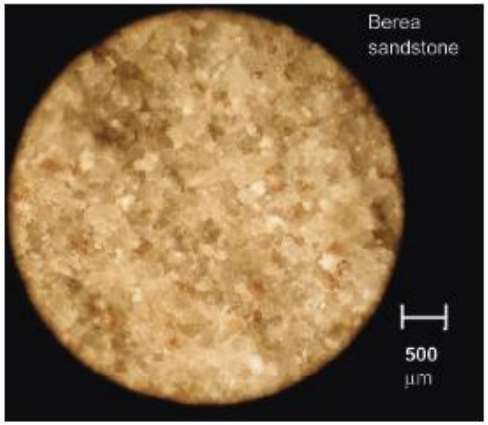
SMARTS is used to study nonlinear mechanical behavior of geomaterials.

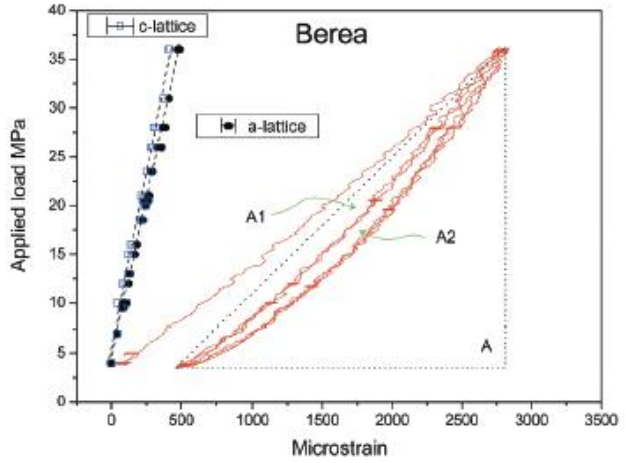




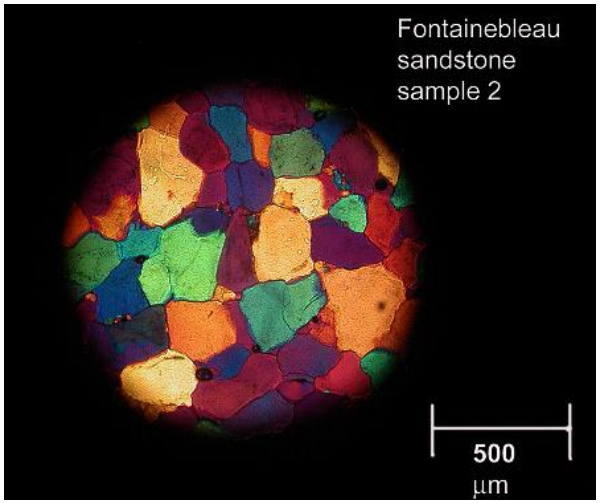


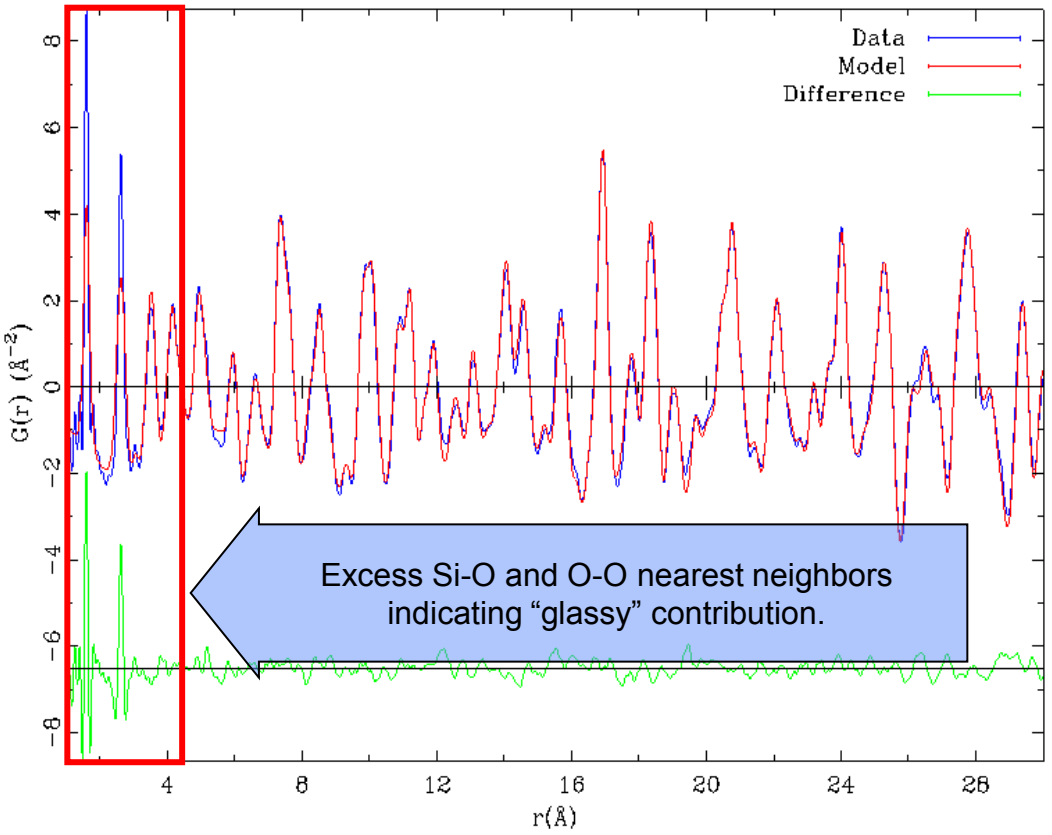






A “glassy” phase in sandstone has been discovered through PDF Measurements on NPDF.





- **Goal: Relate unusual acoustic properties to local atomic structure.**
- **Technique: Pair Distribution Function (PDF) measured on NPDF gives local structural information.**
- **Result: Evidence for a “glassy” phase in Fontainebleau sandstone rock.**

K.L. Page, Th. Proffen, S.E. McLain, T.W. Darling and J.A. TenCate, **Local Atomic Structure of Fontainebleau Sandstone: Evidence for an Amorphous Phase?**, *Geophysical Research Lett.* (2004).

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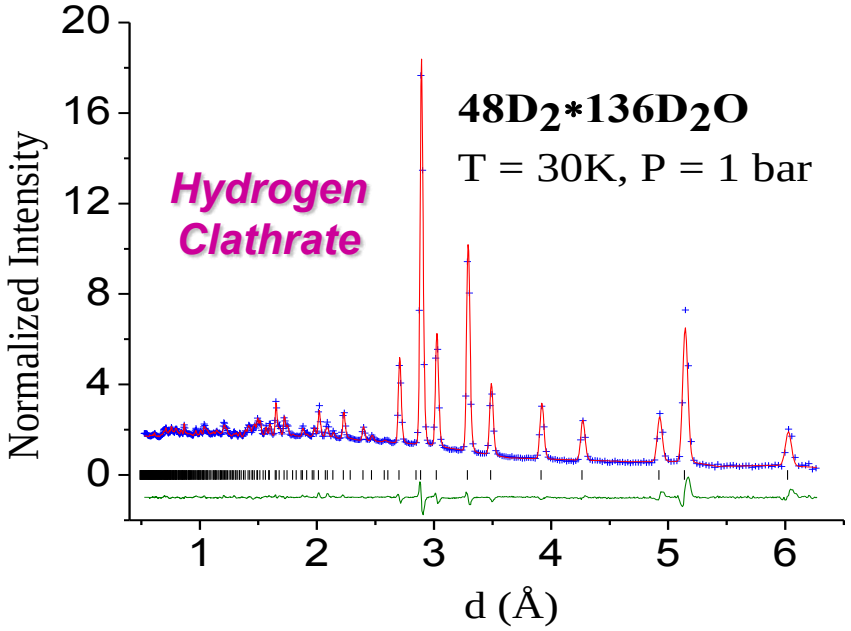
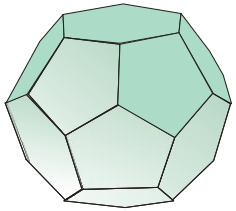
Rietveld refinement of the diffraction patterns



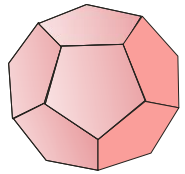
Gas Hydrate (Clathrate) Study

in-situ and *real-time*

neutron diffraction at high-*P* low-*T*



$(5^{12}6^4)$
Hexakaidecahedron



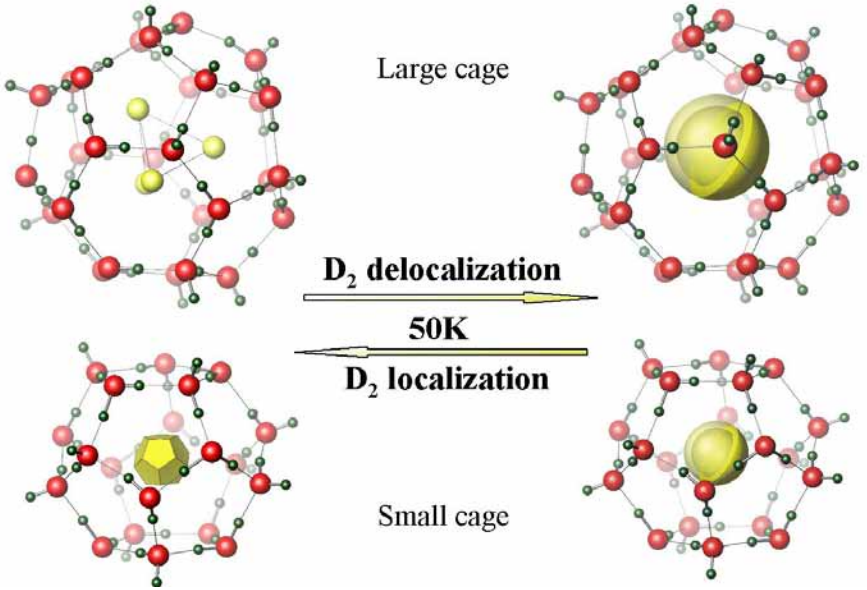
(5^{12})
dodecahedron

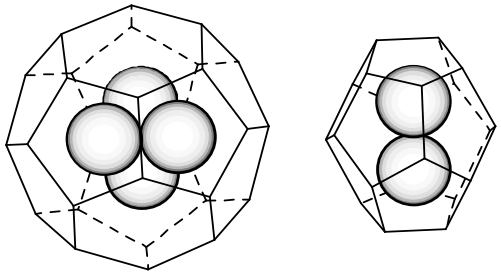
D_2_D_2O sample

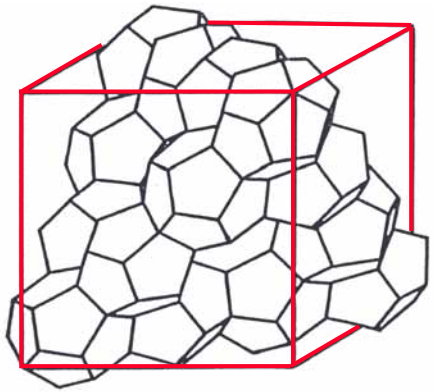
High-P (*up to 200 MPa*) & Low-T (*down to 20K*)

high hydrogen content of up to 45 molar%,

(*Mao et al.*, Science, 2002)







Lokshin et al., PRL (2004)

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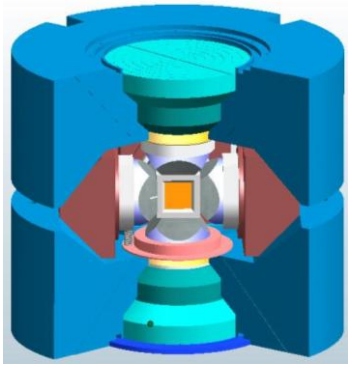
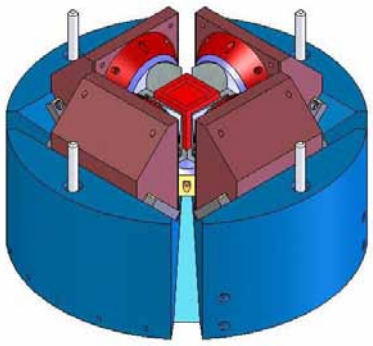
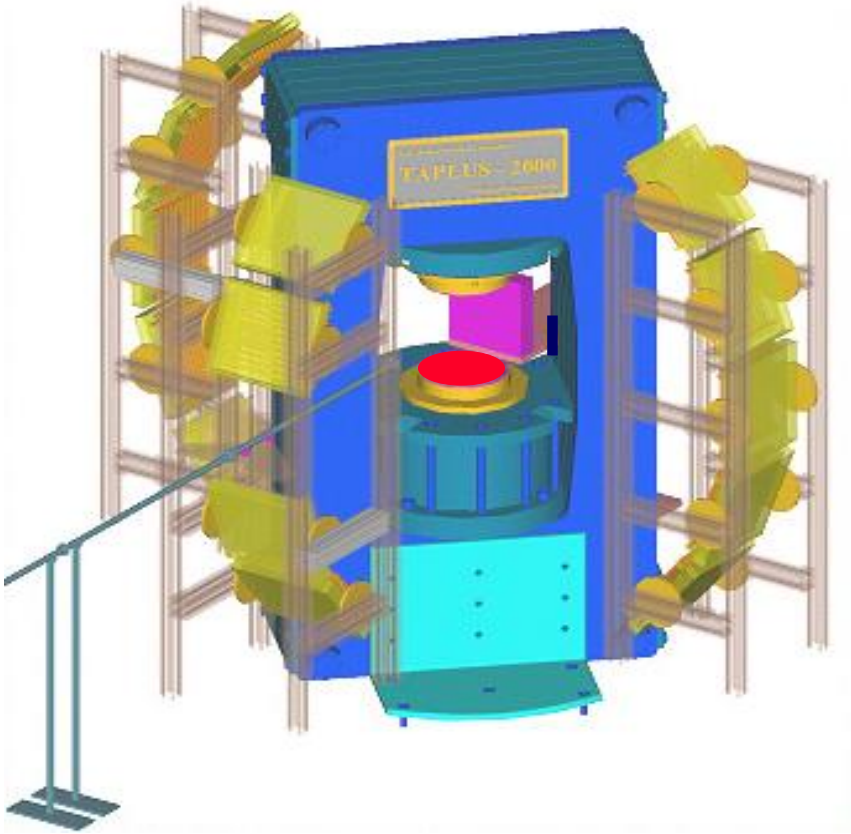
LAPTRON: A proposed instrument for energy materials

high *P-T* diffraction, radiography, ultrasonic, & calorimetry





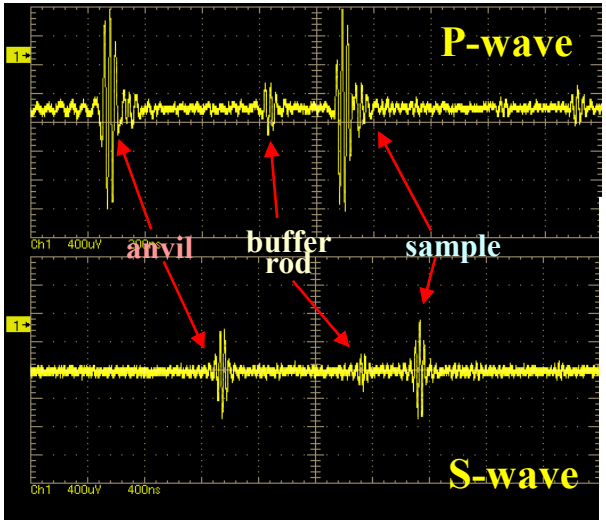


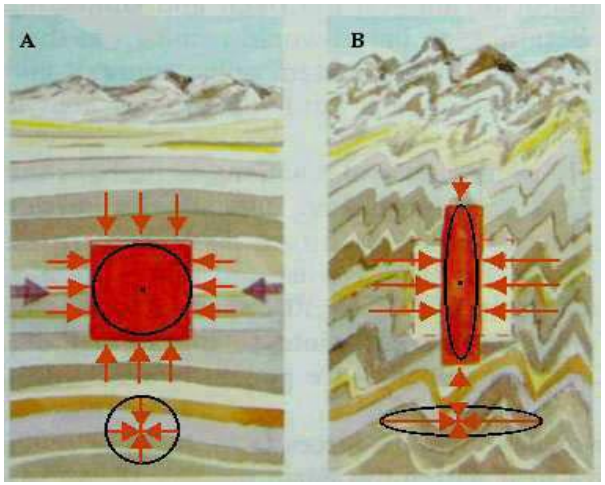
Toroidal anvil package for high *P-T* diffraction and tomography

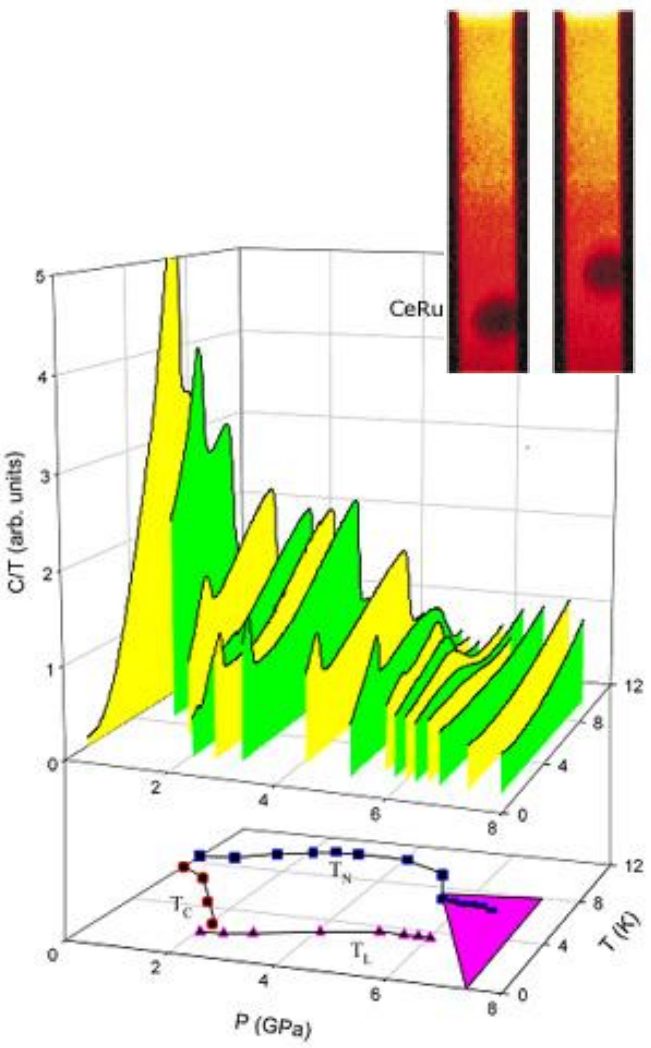
A bearing loading rotation stage to allow 360° sampling at high P-T

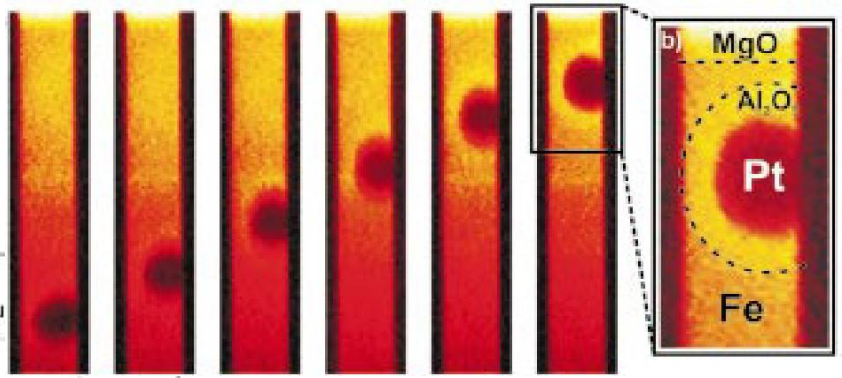
LAPTRON

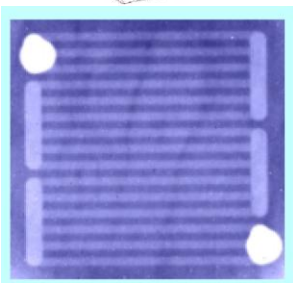
Integration of High *P-T* Neutron Diffraction & *Neutron Radiography/Tomography with Acoustic Elasticity, Thermo-Calorimetry, Deformation Texture/Rheology*

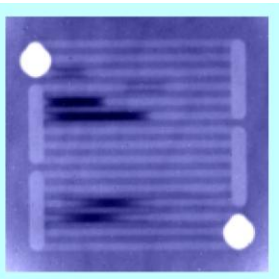






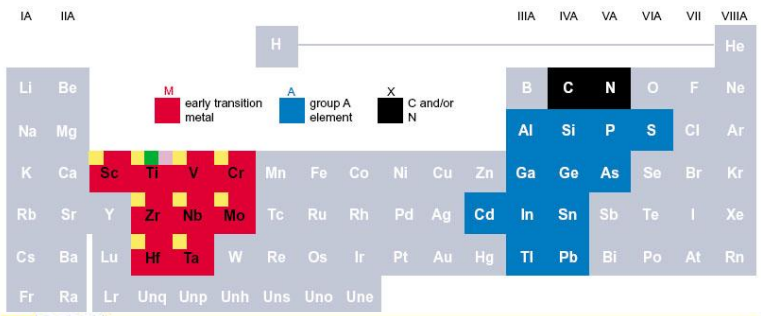






What are MAX Phases?

- MAX are nano-laminated ternary metal carbides, $M_{n+1}AX_n$
- Machinable, ductile, next best thing to self-healing: damage containing
- Doesn't know if it wants to be a metal or a ceramic...
- Many unusual properties (electrical/thermal conductivity, mechanical...)



211

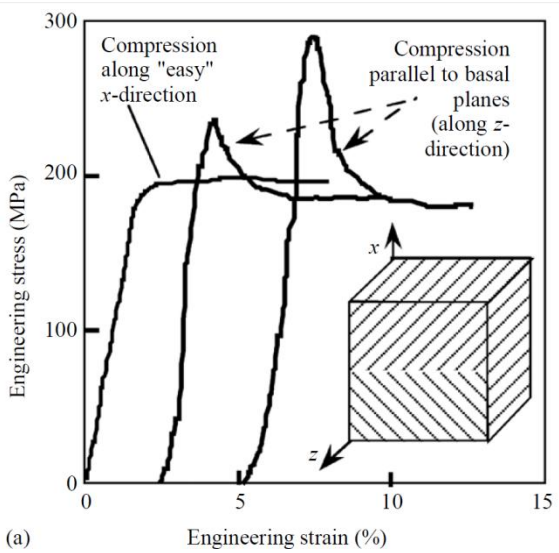
Ti_2AlC^*	Ti_2AlN^*	Hf_2PbC^*	Cr_2GaC	V_2AsC	Ti_2InN
Nb_2AlC^*	$(Nb,Ti)_2AlC^*$	$Ti_2AlN_{0.5}C_{0.5}{}^*$	Nb_2GaC	Nb_2AsC	Zr_2InN
Ti_2GeC^*	Cr_2AlC	Zr_2SC	Mo_2GaC	Ti_2CdC	Hf_2InN
Zr_2SnC^*	Ta_2AlC	Ti_2SC	Ta_2GaC^*	Sc_2InC	Hf_2SnN
Hf_2SnC^*	V_2AlC	Nb_2SC	Ti_2GaN	Ti_2InC	Ti_2TlC
Ti_2SnC^*	V_2PC	Hf_2SC	Cr_2GaN	Zr_2InC	Zr_2TlC
Nb_2SnC^*	Nb_2PC	Ti_2GaC	V_2GaN	Nb_2InC	Hf_2TlC
Zr_2PbC^*	Ti_2PbC^*	V_2GaC	V_2GeC	Hf_2InC	Zr_2TlN

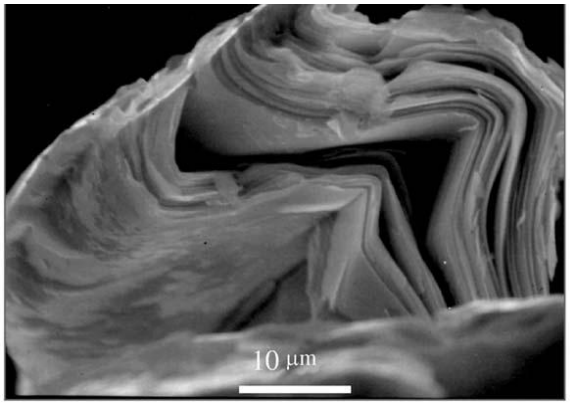
312

$Ti_3AlC_2{}^*$ $Ti_3GeC_2{}^*$ $Ti_3SiC_2{}^*$

413

$Ti_4AlN_3{}^*$



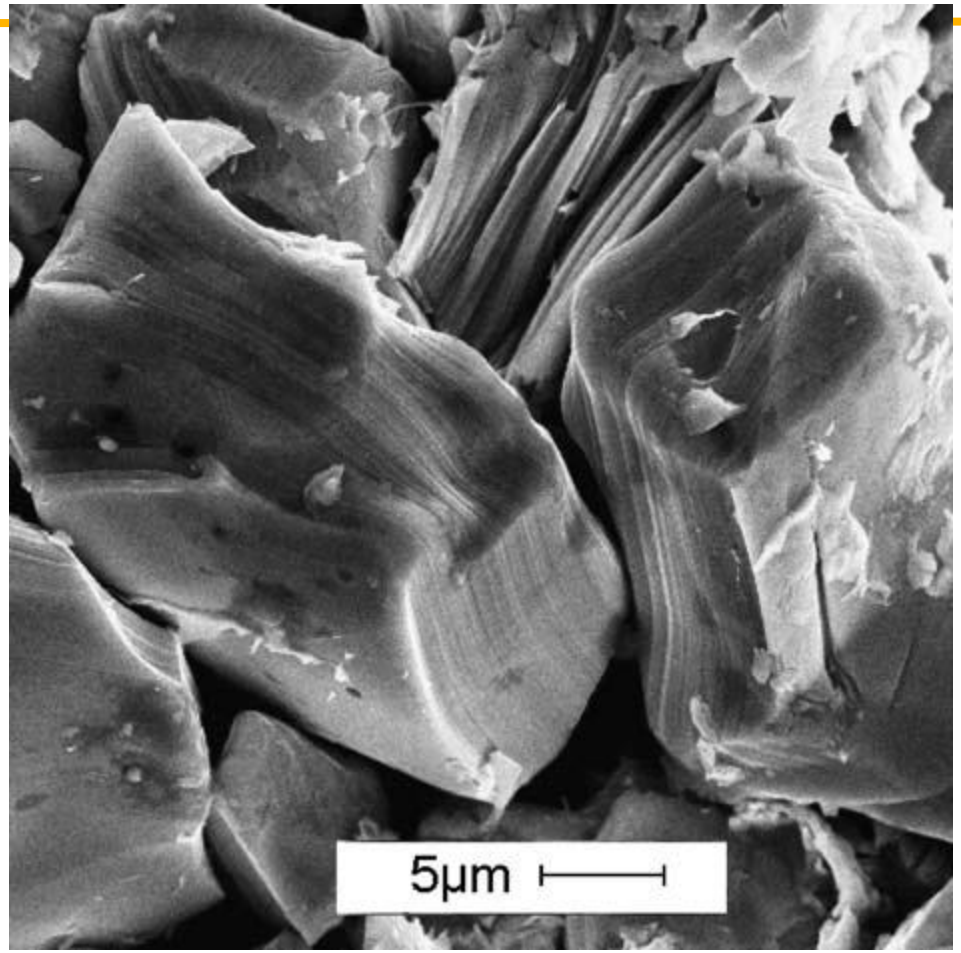


Ti_3SiC_2 hit with a hammer

LANSCE Los Alamos Neutron Science Center

Drexel UNIVERSITY

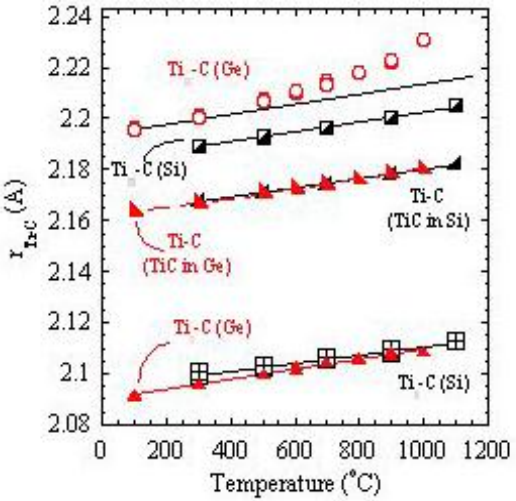
Mystery: Why does Ti_3GeC_2 exhibit dramatic damping in ultrasound measurements at ~450C?

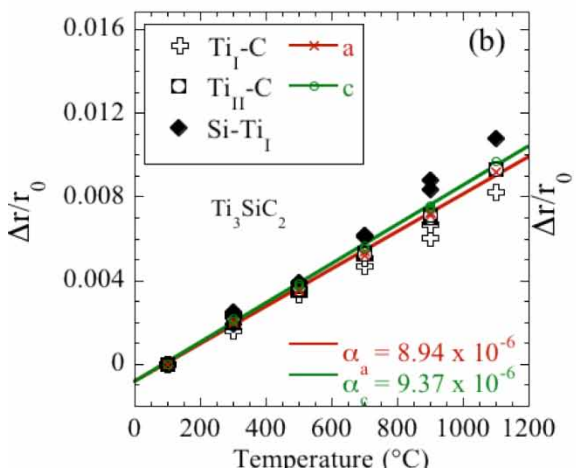


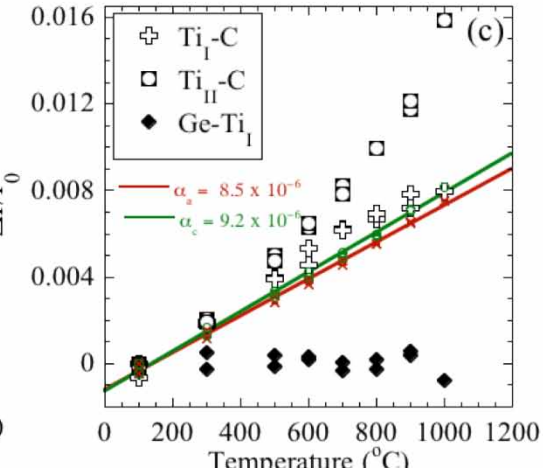
Michel Barsoum, Drexel Univ
nature materials | **VOL 2 | 107 FEBRUARY 2003**

Results: Bond lengths

- Ti-C bond in Ti_3GeC_2 deviates from linear behavior of all other Ti-C bonds

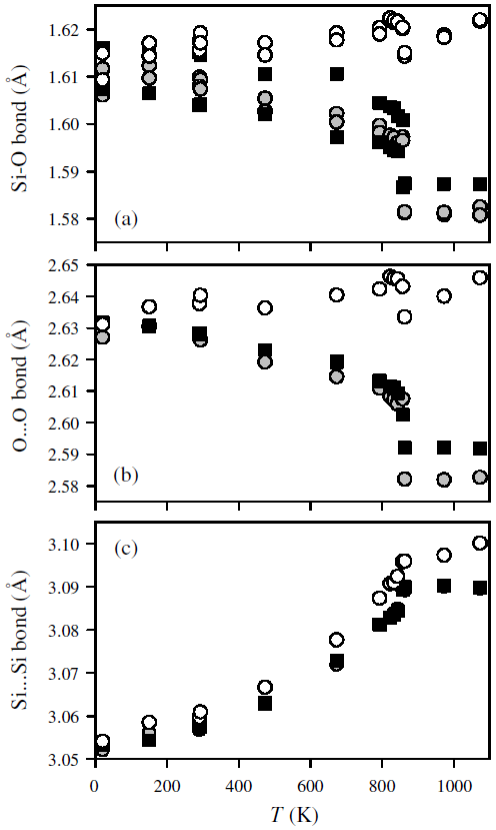


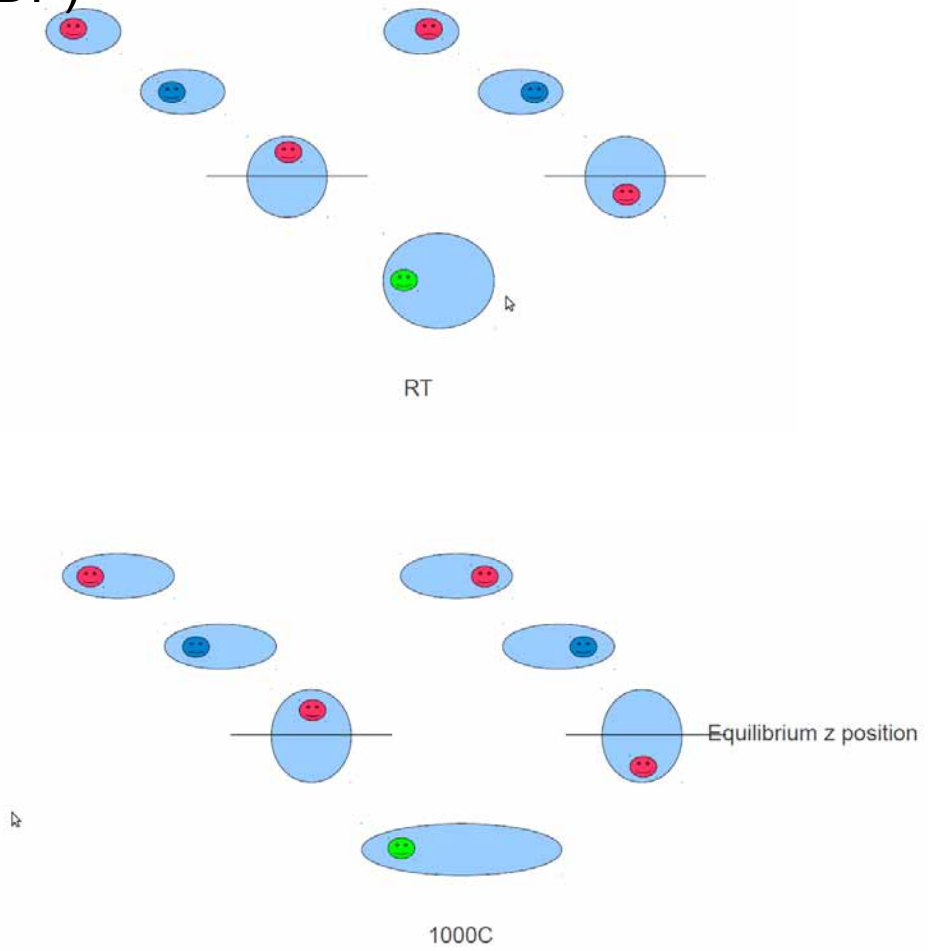




Results: Possible explanation for bond-lengths anomaly

- Correlated motion was found as in quartz
- Explanation is difference between average bond length (Rietveld) and instantaneous bond length (PDF)

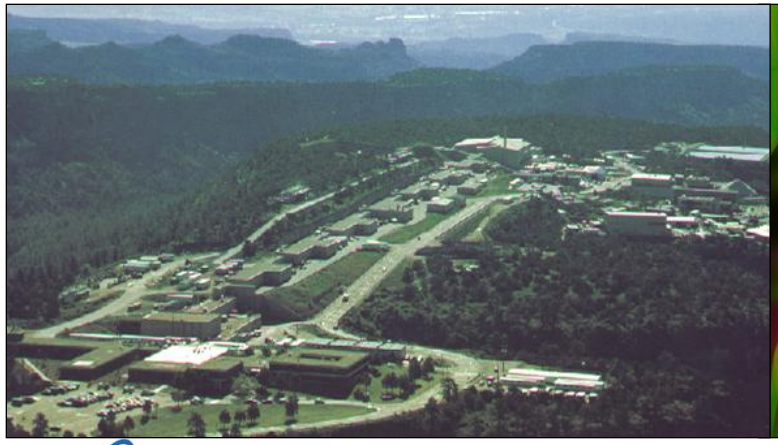




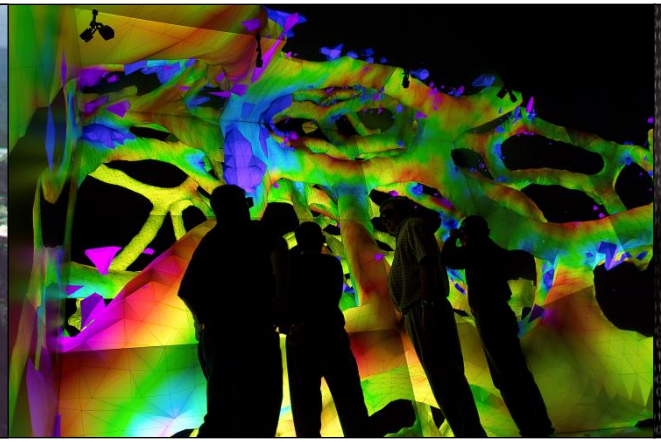
Los Alamos science in the 21st century

Los Alamos as the Premier National Security Science Laboratory will solve problems that:

- **Are large scale, complex, and high impact;**
- **Require multidisciplinary science, technology, and engineering;**
- **Utilize unique, multifaceted, or large experimental facilities;**
- **Depend on fundamental research and development; and**
- **Develop technology that is highly complex, and sensitive or classified nature.**

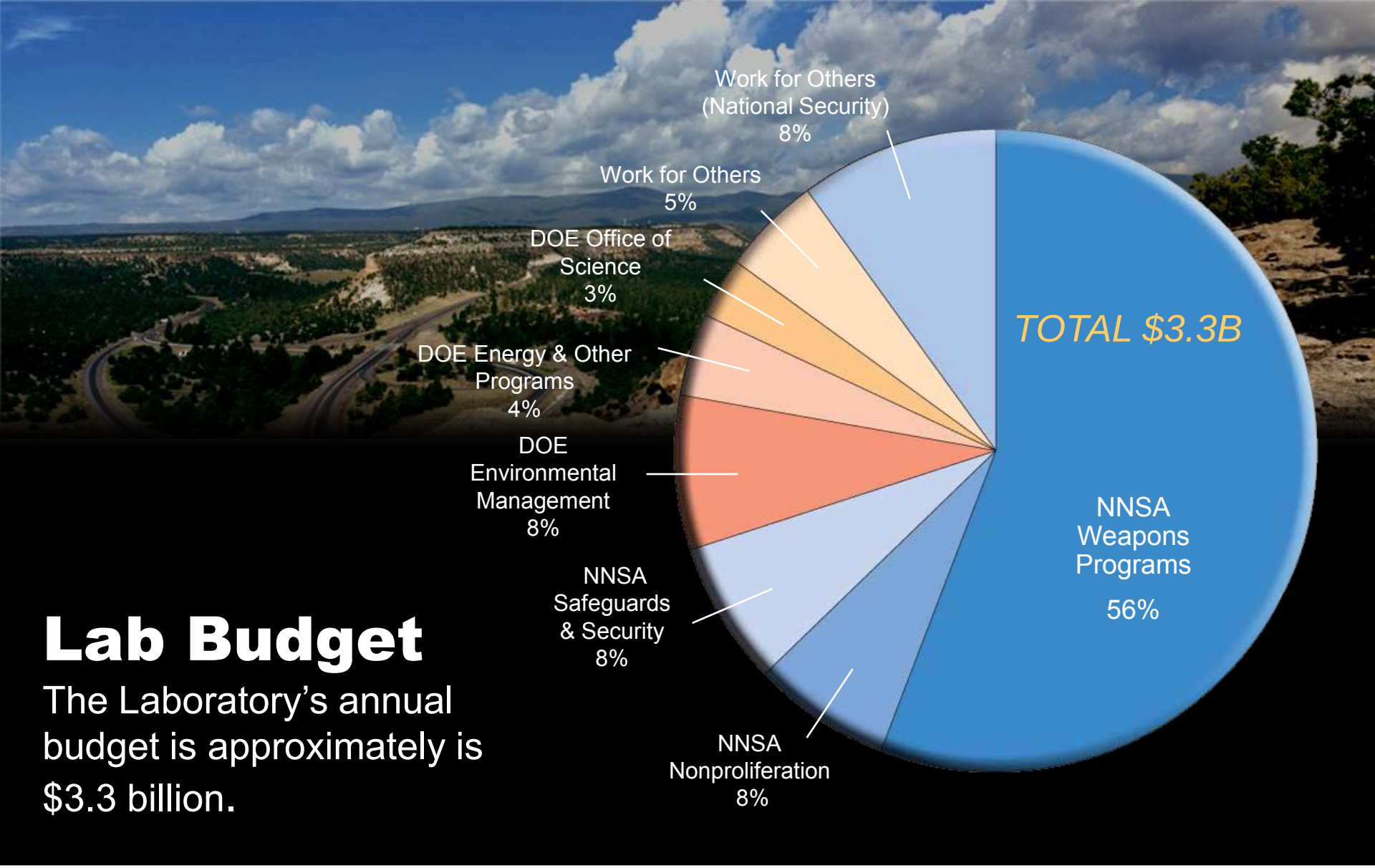


LANSCE



Immersive Visualization Cave

High Throughput Laboratory Network



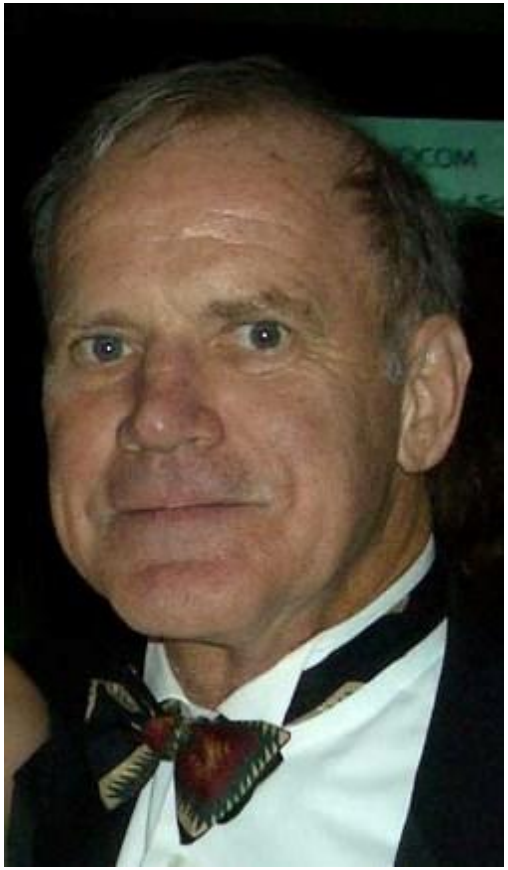
Lab Budget

The Laboratory's annual budget is approximately is $3.3 billion.

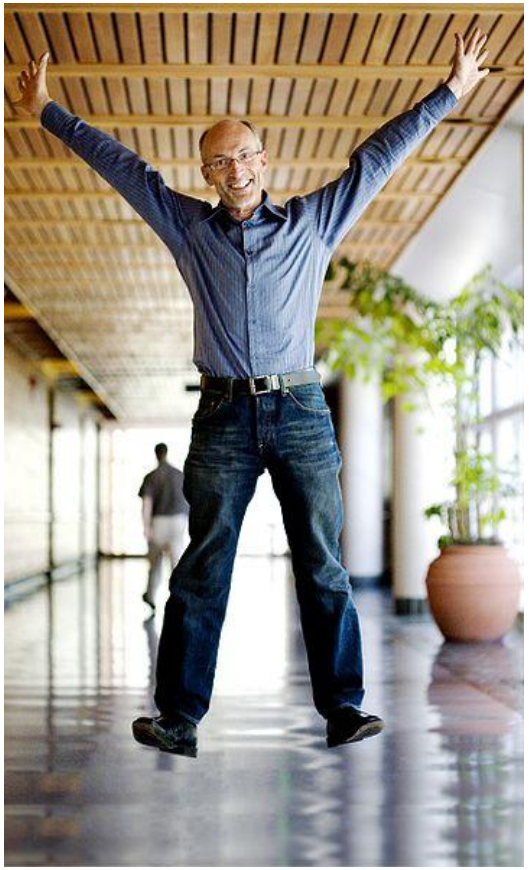
Quick Poll

Who is the greatest living person?

Greatest Living Person?



Kary Mullis, PCR (1993)



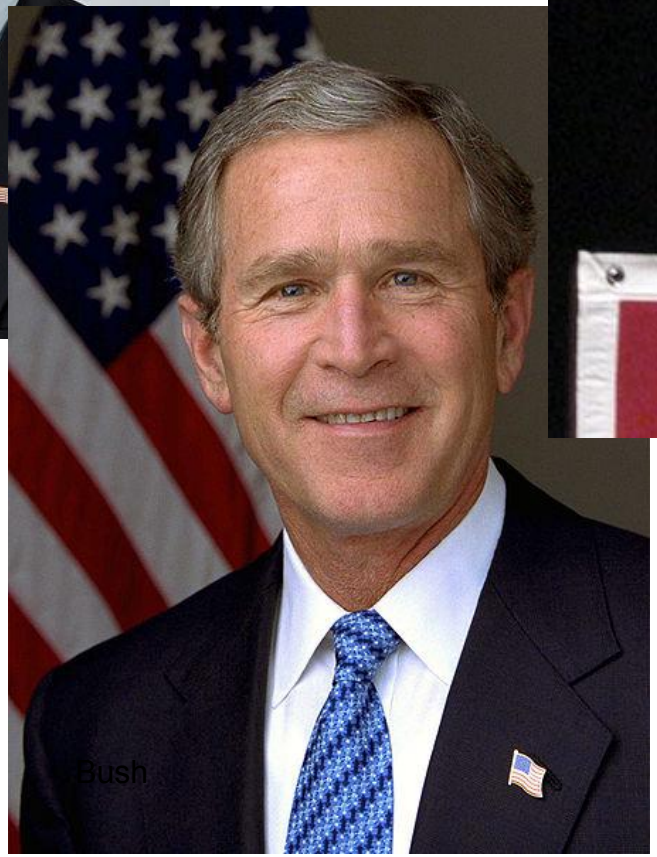
Stuart Parkin, GMR apps

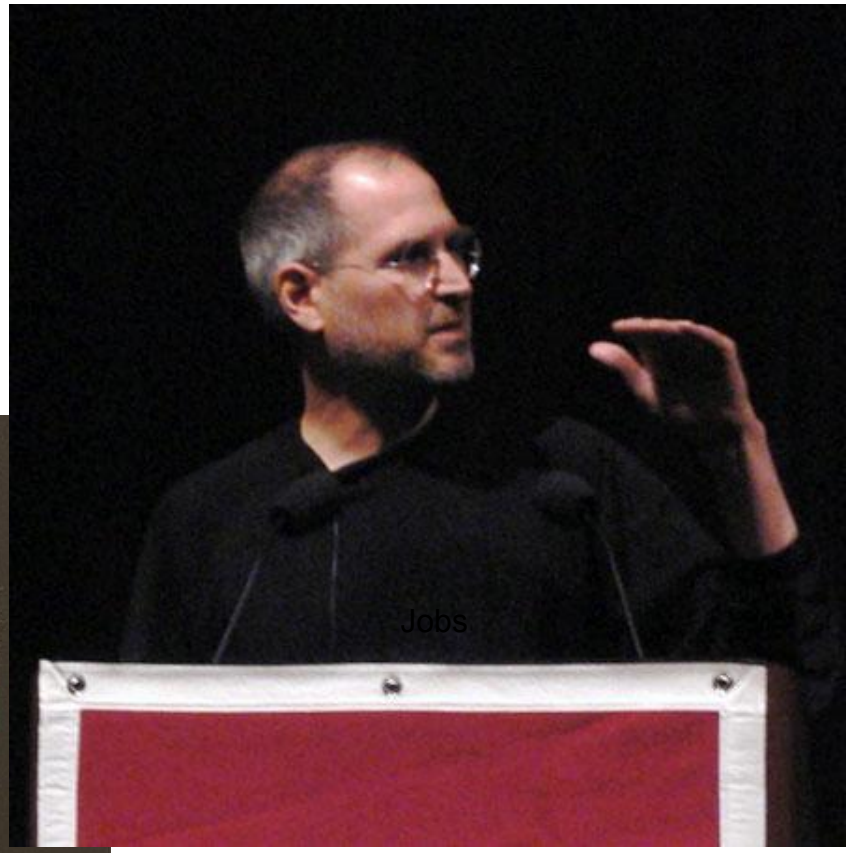
Ada Yonath, Weizmann
Chemistry Nobel 2009

TIME 100

Seven time honoree Oprah Winfrey

...not six-timers!





Four-timers

"When I compare our high schools to what I see when I'm traveling abroad, I am terrified for our workforce of tomorrow."

–Four x TIME100 Bill Gates, Chairman and Chief Software Architect of Microsoft Corporation

Albuquerque, 1976

Highest physicist on TIME 100

Three-timer Angela Markel, Chancellor of Germany

Summary

- Making neutrons
- Using neutrons and why
- User Facilities
- Success stories

Using neutron scattering gives you a competitive advantage in your research.

Louie Rosen June 10, 1918-August 20, 2009