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Title: Achieving Materials functionality Designing & Assessing

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Intended for: WPI Lectures for undergrad students on material research.

Achieving Materials Functionality
Designing & Assessing

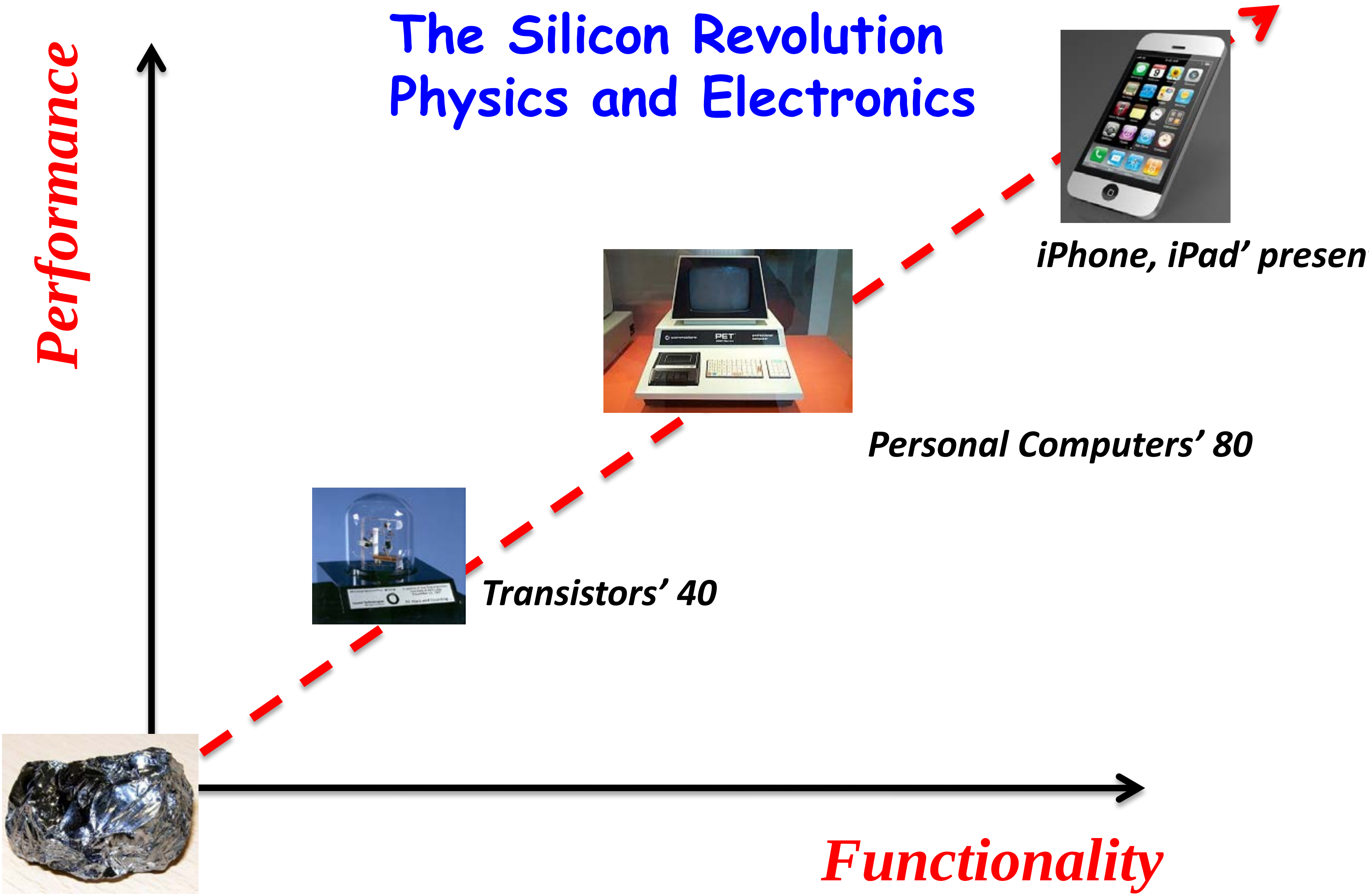
MATERIALS RESEARCH

Making – Measuring – Assessing - Applying

The Good, the Bad and the "Interesting" of Experimental Sciences

Materials Science: *Why is this Important*

The Silicon Revolution
Physics and Electronics

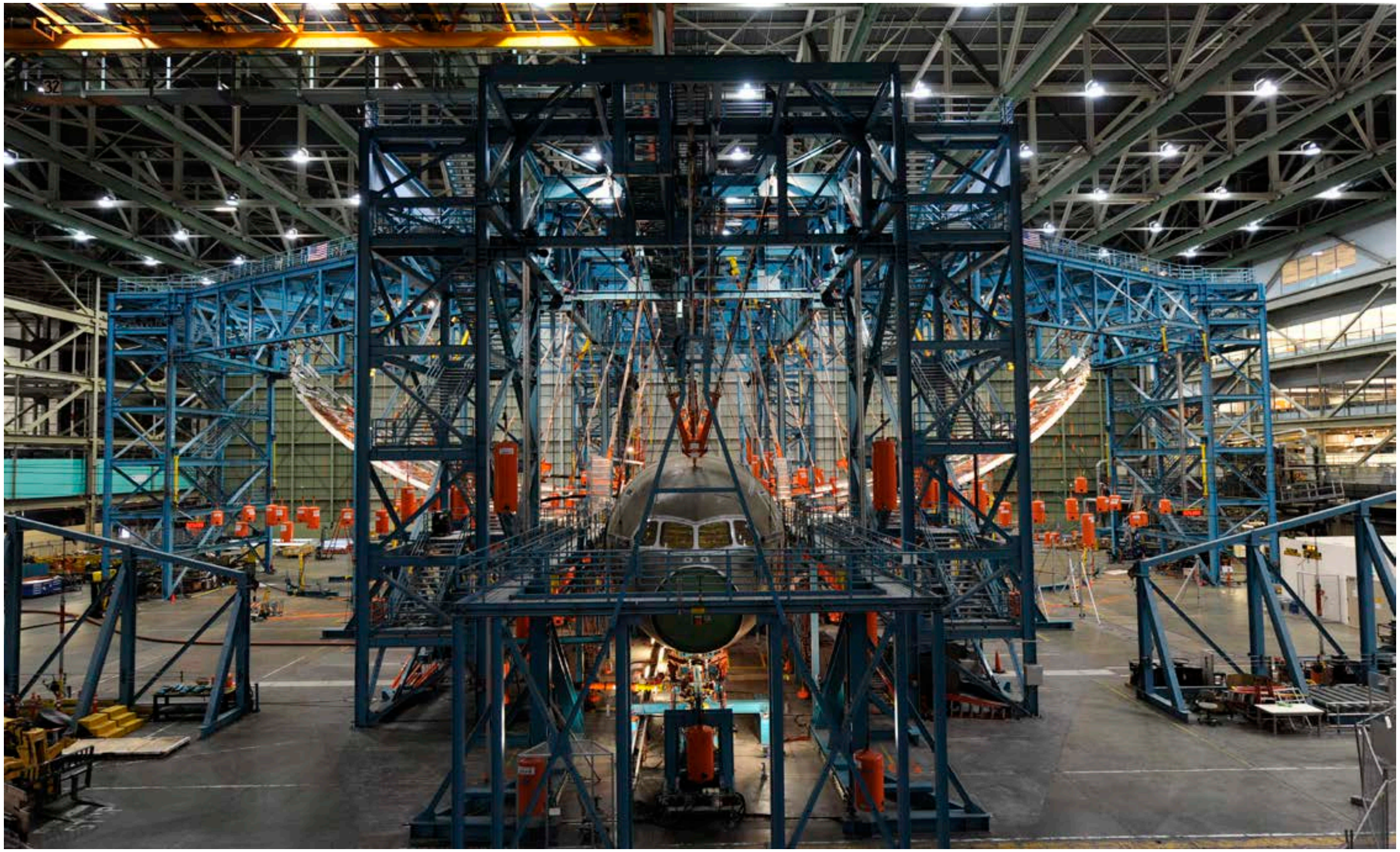


Silicon: Eighth most common element in the universe

Achieving Materials Functionality

Designing

Achieving Materials Functionality
Assessing



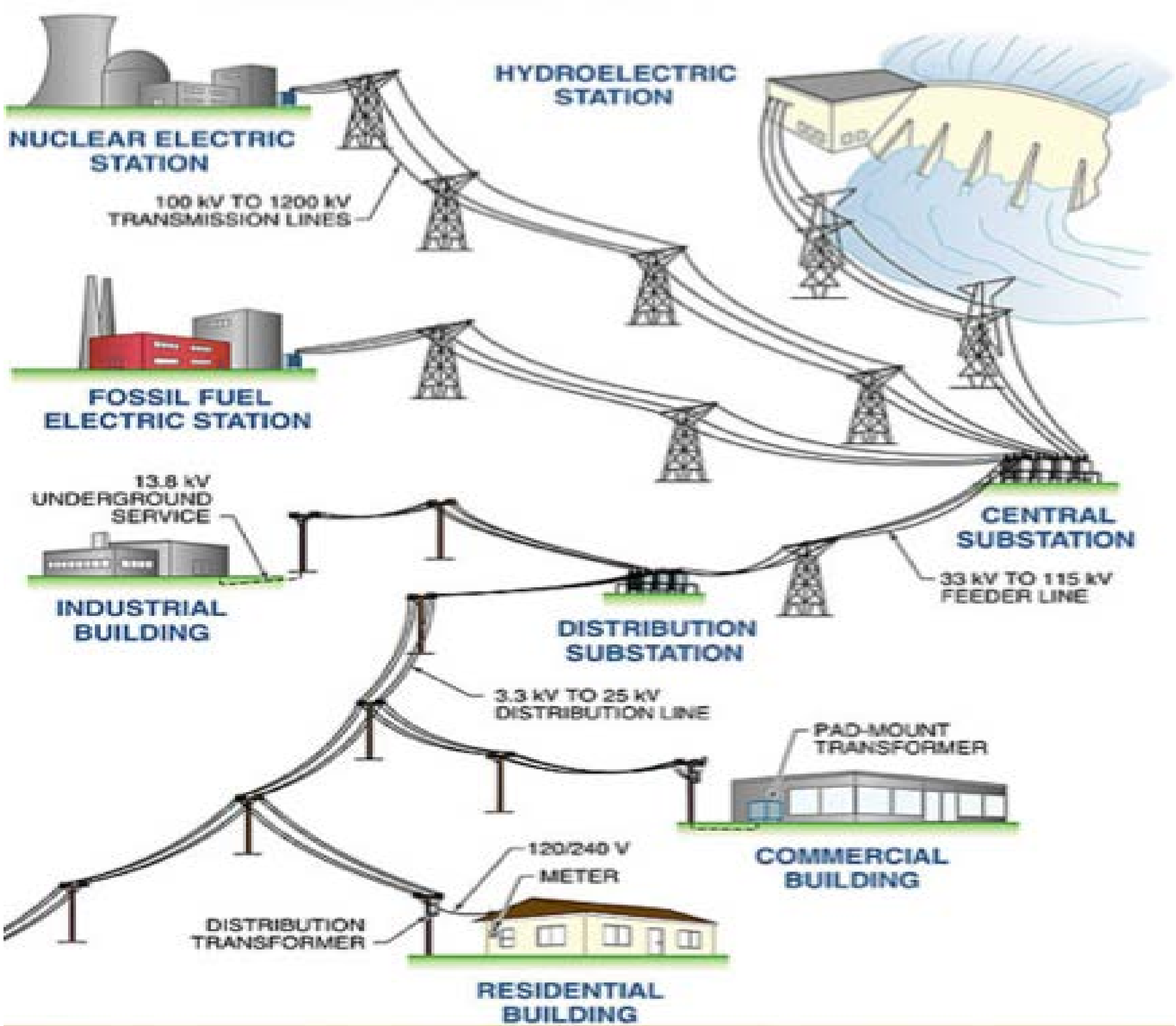
During the test, the wings on the 787 were **flexed upward "approximately 25 feet"** which **equates to 150 percent of the most extreme forces the airplane is ever expected to encounter during normal operation.**

So What?

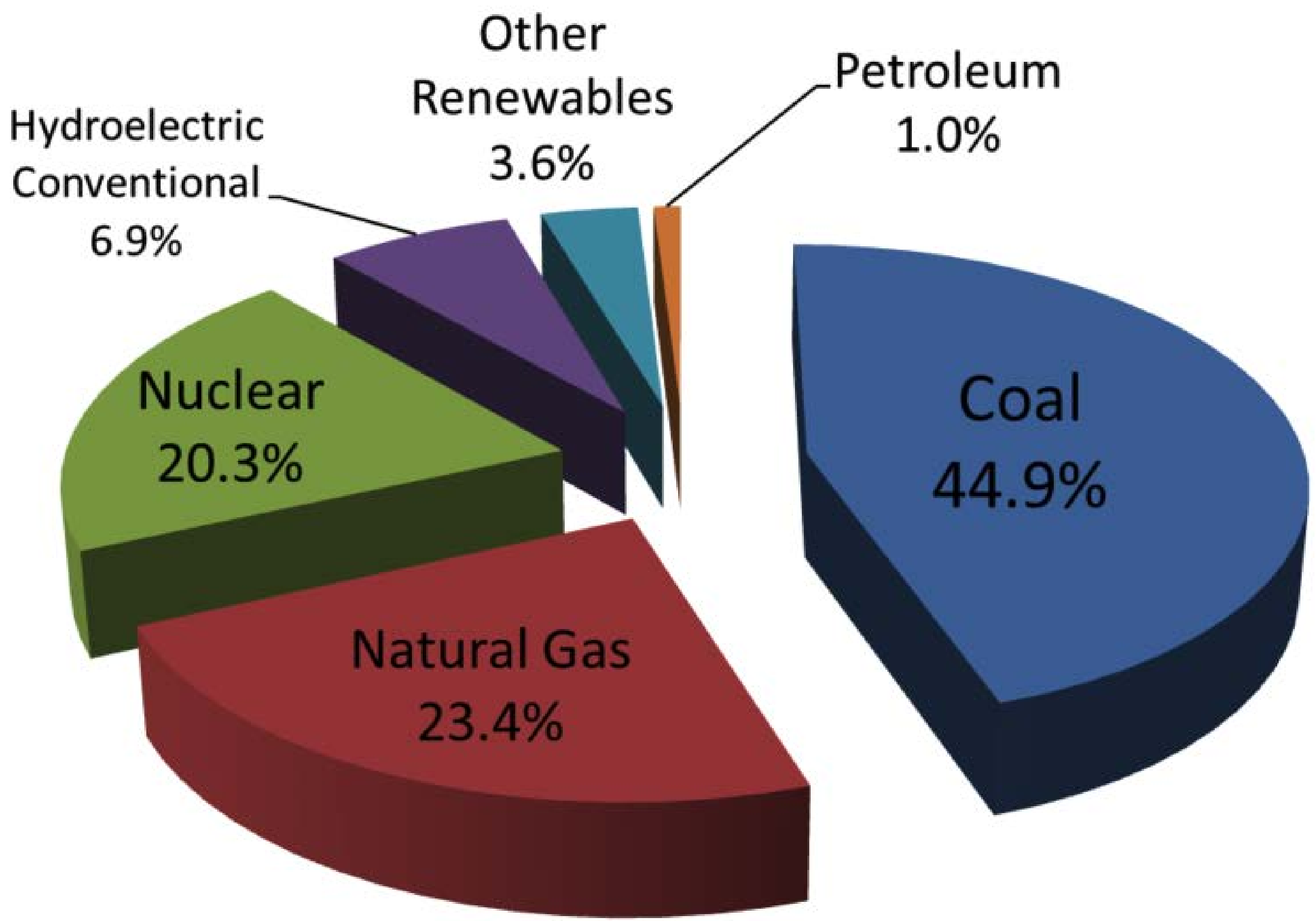
The Electrical Grid - The Triumph of 20th Century Engineering

Clean, versatile electric power, basically everywhere

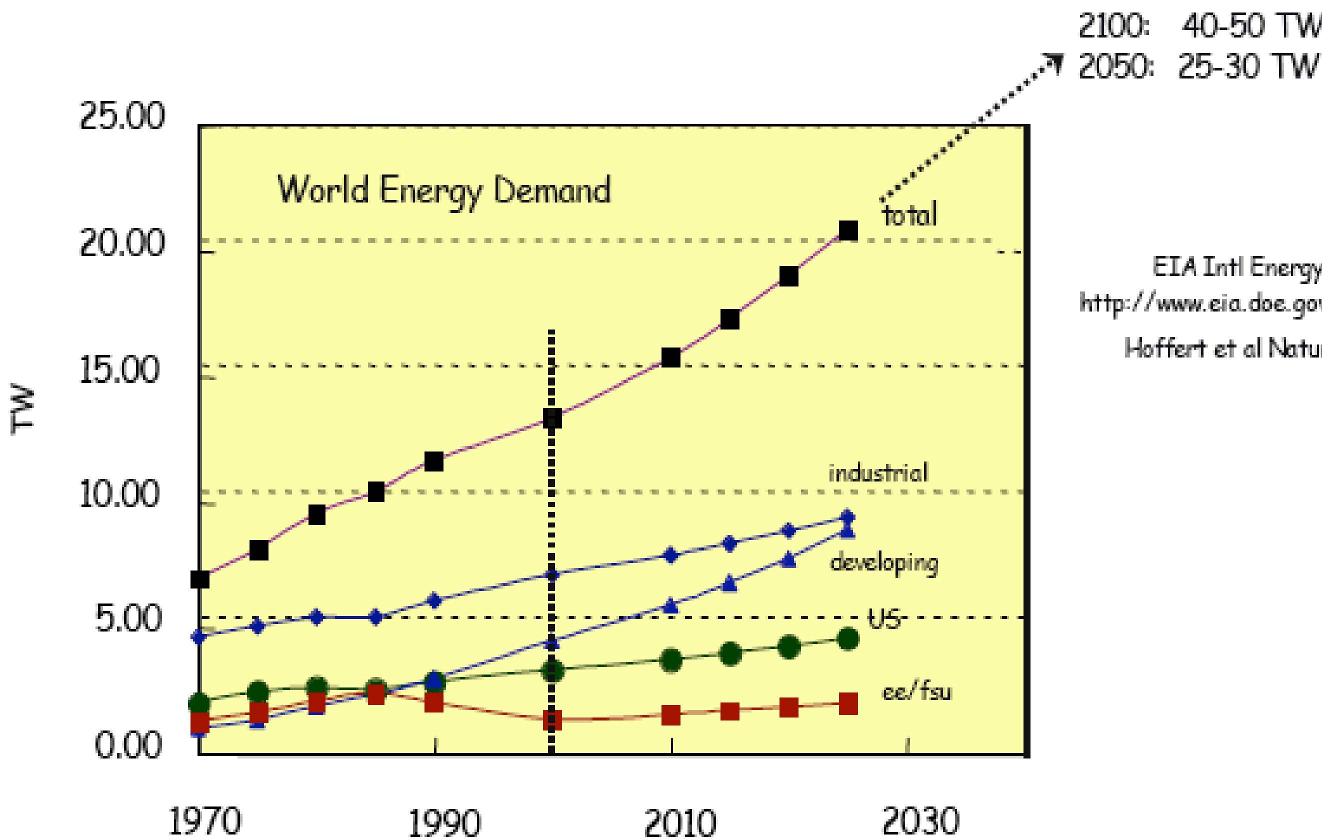
Electricity production and distribution…main core is still the same



2009 U.S. Electricity Generation by Source



The Energy Challenge



EIA Intl Energy Outlook 2004
http://www.eia.doe.gov/oiaf/ieo/index.html
Hoffert et al Nature 395, 883,1998

Double demand by 2050

Triple demand by 2100

Challenge for production, delivery and use

The 21st Century: A Different Set of Challenges

capacity

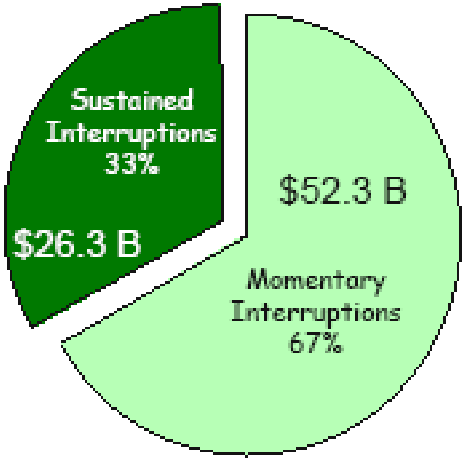
growing electricity uses
growing cities and suburbs
high people / power density
urban power bottleneck

2030
50% demand growth (US)
100% demand growth (world)

reliability
power quality

average
power loss/customer
(min/yr)

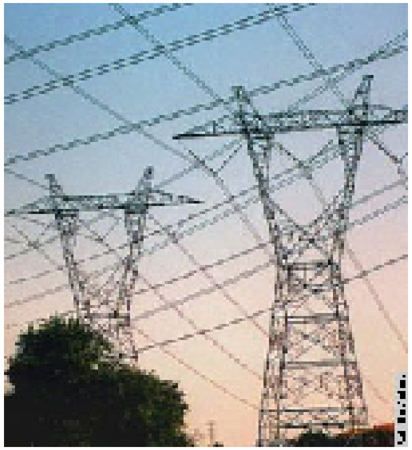
US	214
France	53
Japan	6



$79 B economic loss (US)

LaCommare & Eto, Energy 31, 1845 (2006)

efficiency
lost energy



62% energy lost in production / delivery

8-10% lost in grid

40 GW lost (US)
~ 40 power plants

2030: 60 GW lost
340 Mtons CO_2

…But the cost!!!

Country	Annual CO_2 Emissions (In thousands of metric tons)	Percent of global total	% of World Population	Per Capita (Metric ton)
China	6,103,493	21.5%	19.6%	4.62
USA	**5,752,289**	**20.2%**	**4.5%**	**18.99**
EU	3,914,359	13.8 %	3.5%	8.07
Russia	1,564,669	5.5%	2.1%	10.92
India	1,510,351	5.3%	17.3%	1.31
Brazil	352,524	1.2 %	2.8%	1.86

We need solutions and *fast*

….Have I scared you yet…
Hope NOT!

Alternatives

- Hydroelectric power
- Geothermal
- Bioenergy
- **Nuclear fission**
- Wind energy
- **Solar energy**

The New Frontier of Materials Research

From "Observation & Validation"

To Predict and Control

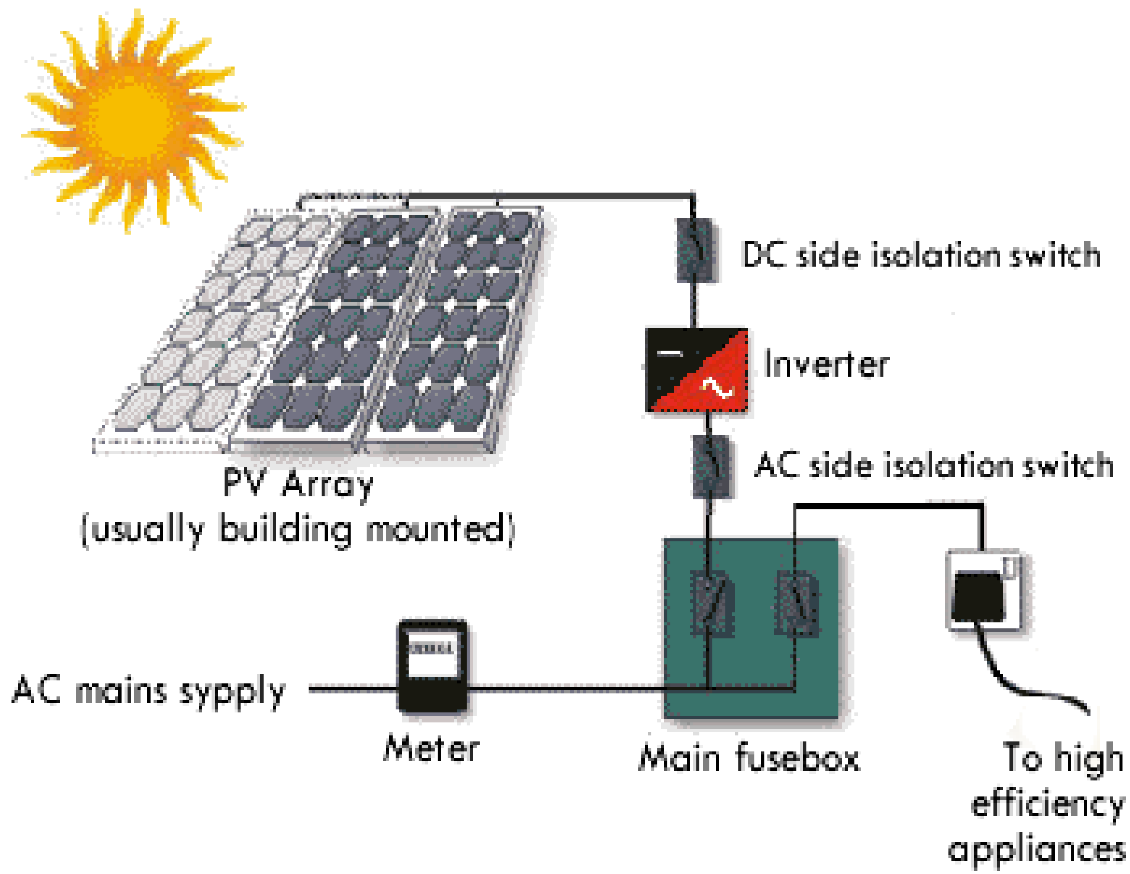
What this really means….

Materials for Energy Conversion, Storage and Transmission

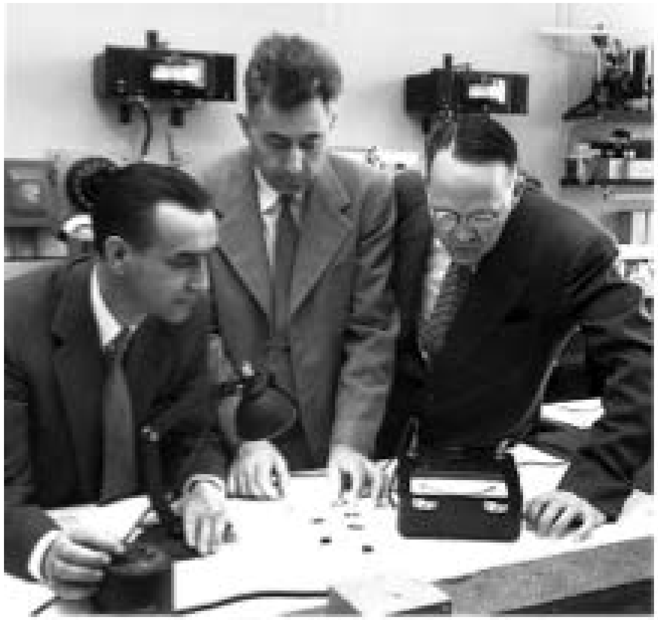
Solar Energy

Perhaps…One of the most talked-about alternative energy sources…

Sun’s rays “heat” and “light”. Heat used in thermal systems (e.g. sterling engines)…”light” ***photovoltaic (PV) systems***; converting light to electricity….PV array (silicon material or???`



Photovoltaic Systems

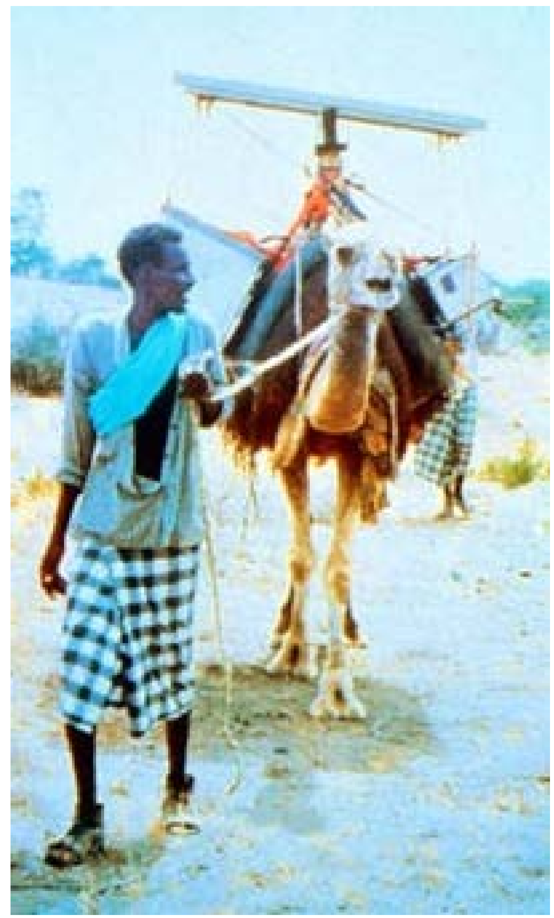


Lucent Technologies Inc./Bell Labs

First observation of PV effect in silicon solar cells (1954 by Pearson, Chapin, and Fuller at AT&T Bell Labs)

DOE/NREL, NASA/Smithsonian Institution/ Lockheed Corp.

PV: satellite and spacecraft since 1958 for power generation.



PV panels and small refrigerators

PV Effect

Light (***= photon***) interacts with a material surface, the electrons present in the valance band of the metallic atom absorbs energy and, being excited, jump to conduction band and become free.

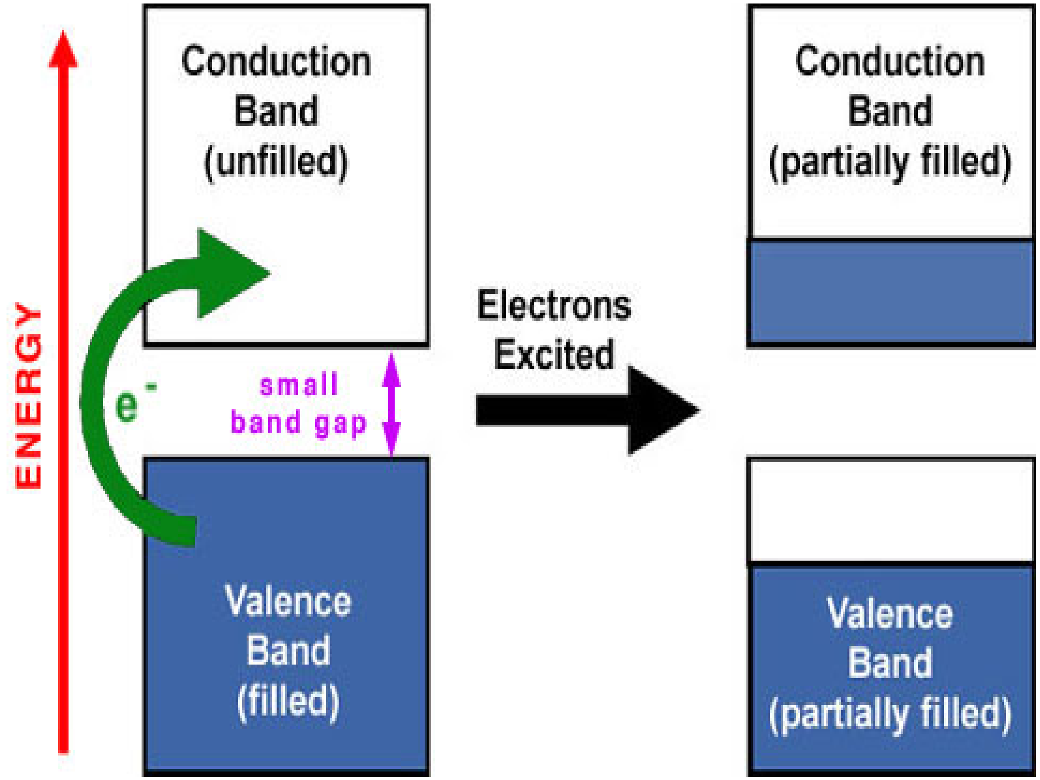
The **"photovoltaic effect"** is the basic physical process through which a solar cell converts sunlight into electricity. Discovered by a French experimental physicist (*Edmund Becquerel; "La Lumière, ses causes et ses effets*") in 1839 when he was 20. Becquerel found that certain materials would produce small amounts of electric current when exposed to light.

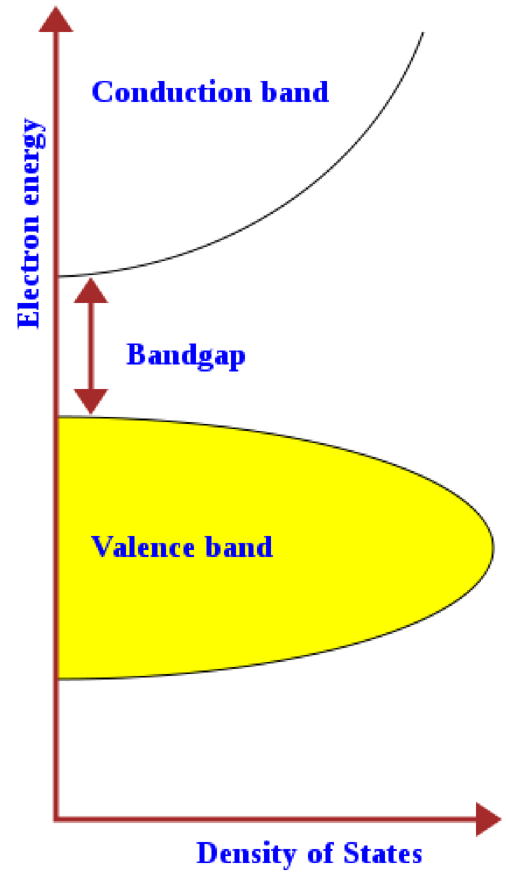
When photons strike a **solar cell**.. may be reflected or absorbed, or they may pass right through. When a photon is absorbed, the energy of the photon is transferred to an electron in an atom of the cell (***which is actually a semiconductor***).

NOTE: **Photovoltaic effect** differs from **Photoelectric effect** in that electrons are transferred between different bands (i.e., from the valence to conduction bands within the material).

The concept of energy bands in metals/solids

In a solid, the valence band is the highest range of electron energies in which electrons are bound to atoms….

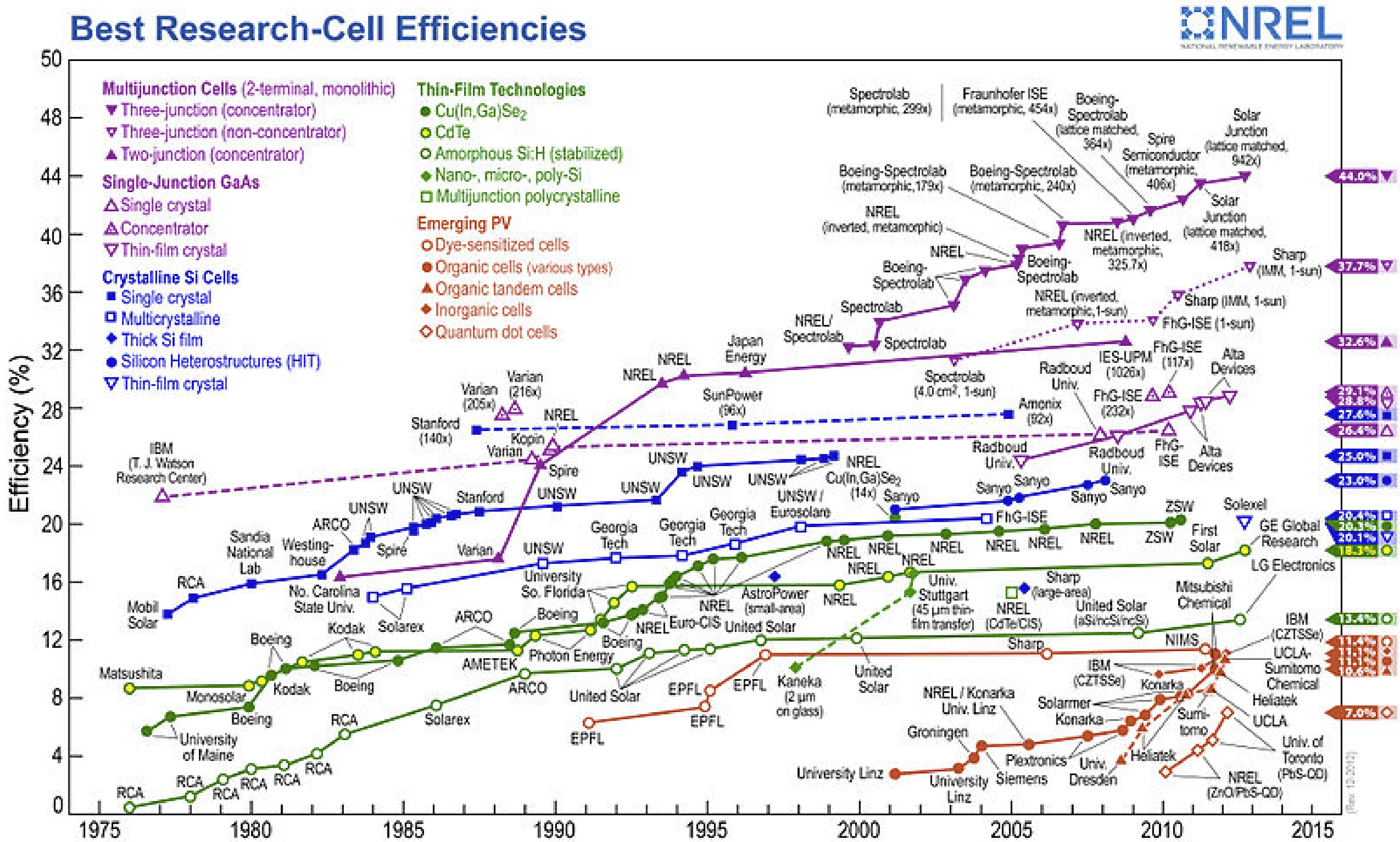




The Fermi level is a hypothetical level of potential energy for an electron inside a crystalline solid

Research: Combination of Hard Work, Dedication, and Continuing Investment….*and takes time too*

Reported timeline of solar cell energy conversion efficiencies (from National Renewable Energy Laboratory (NREL)



High Power Electricity Transmission

Lost in Transmission

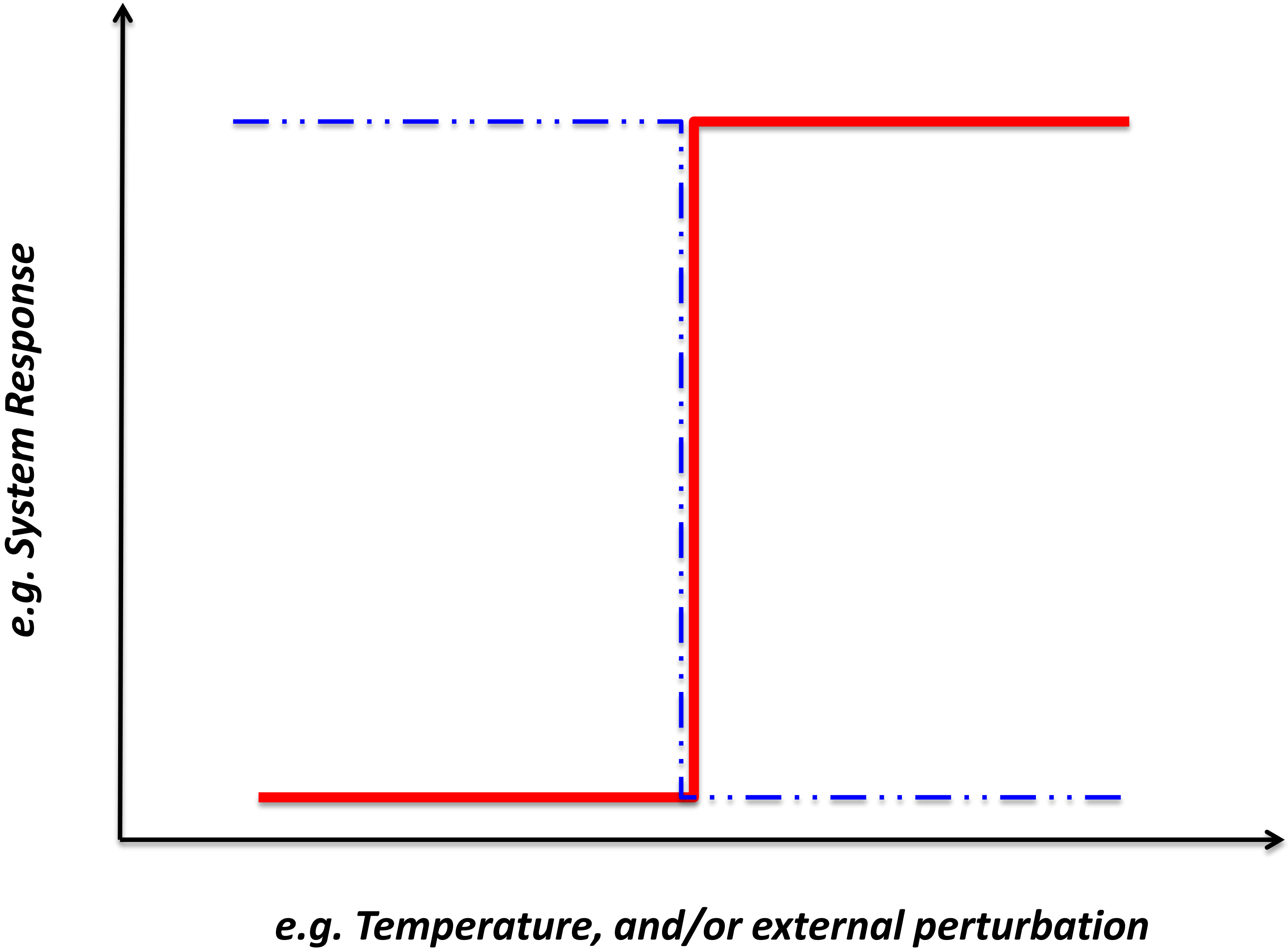
Saving Energy with Superconductivity

Electrical Power Transmission: Some of the problem…aging infrastructure

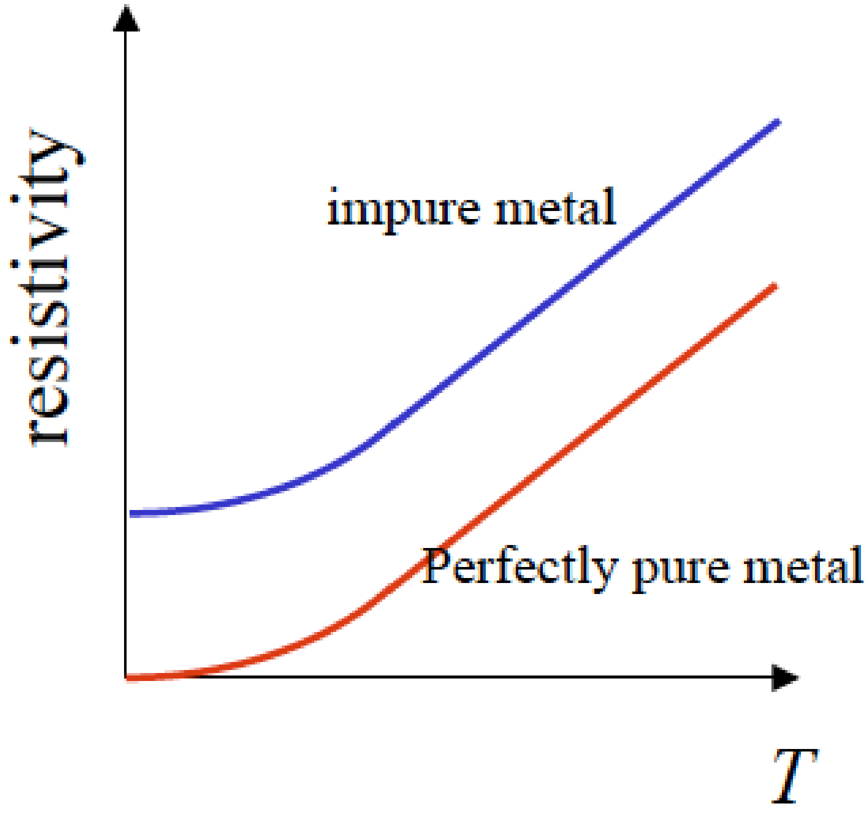
1913 subterranean rats' nest beneath Wall Street… amazingly, looks much the same today as it did a century ago.

Credit: 1913 image

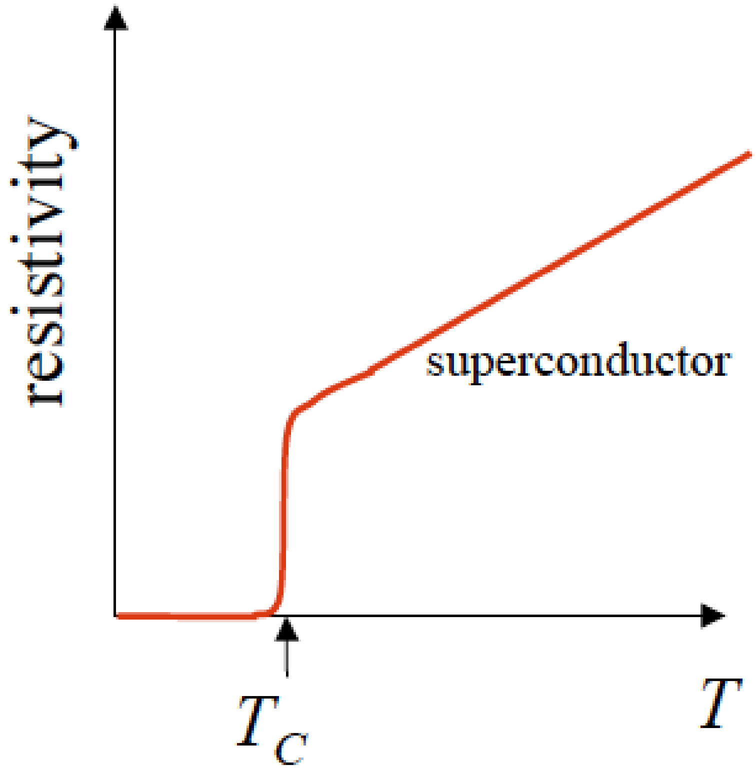
Modernizing Electricity Transmission: The Concept of Superconductivity



Electrical Resistivity: Metals



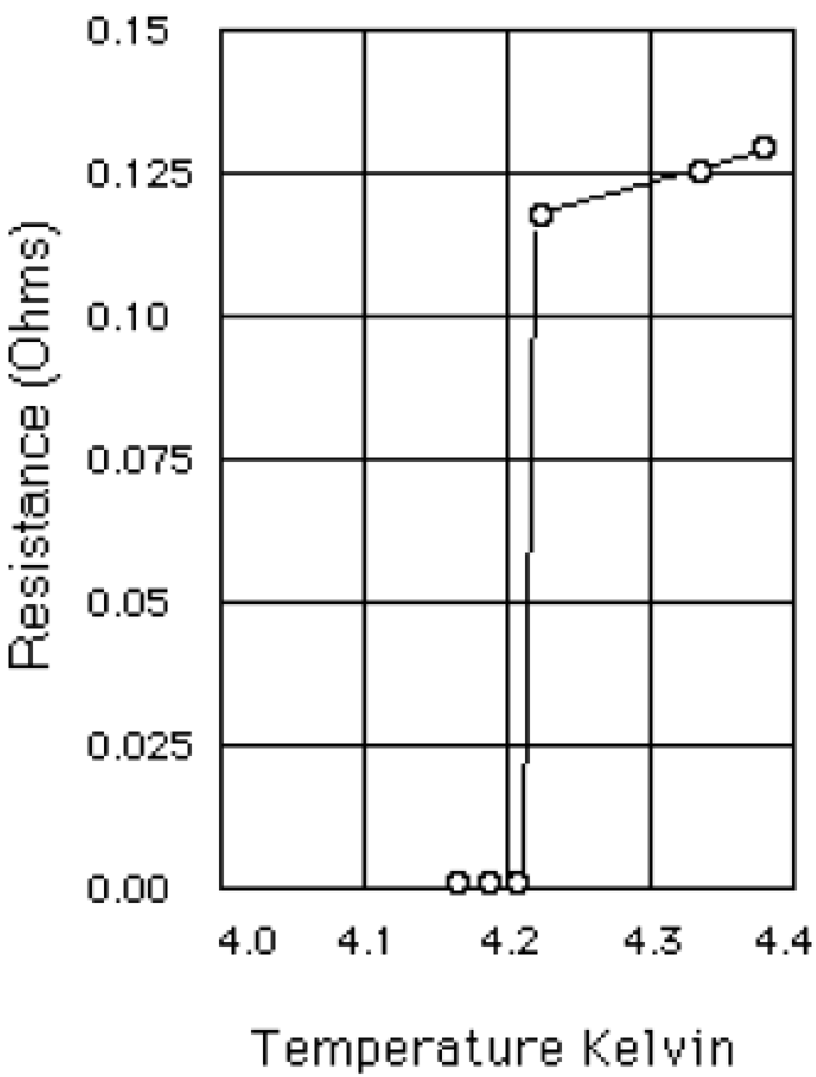
Residual resistivity ρ_0

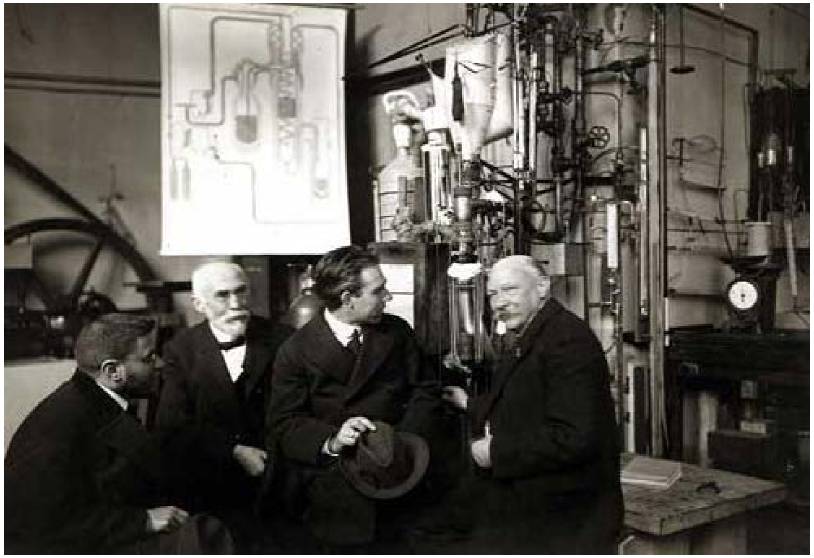


Critical temperature

transition temperature

Discovery of Superconductivity

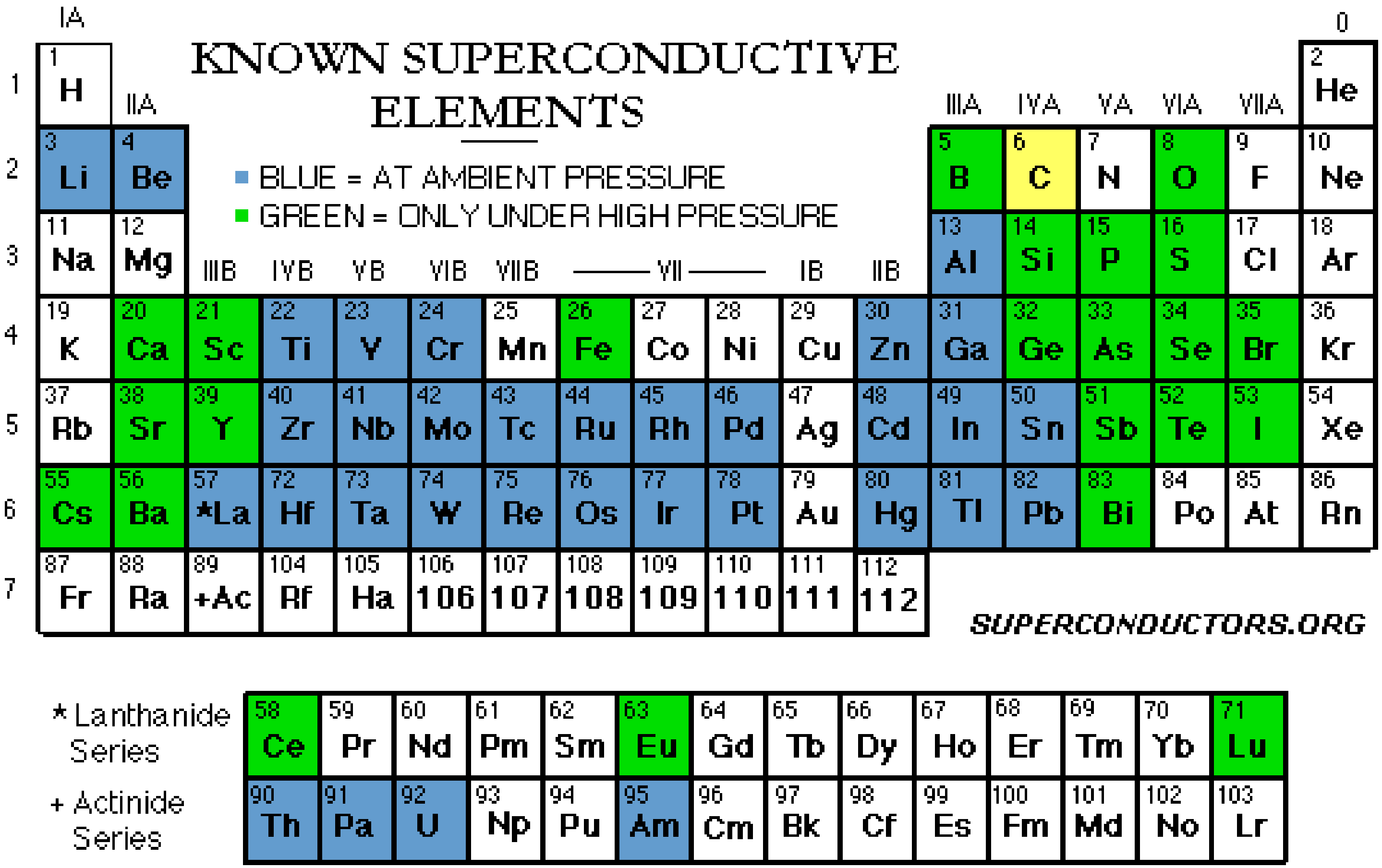




Ehrenfest, Lorentz, Bohr, and Onnes (1908/11)

Heike Kamerlingh Onnes (Leiden, The Netherlands) discovered superconductivity – April 1911. He was studying the resistance of solid mercury at cryogenic temperatures using the recently-produced liquid helium as a refrigerant. At the temperature of 4.2K, he observed that the resistance abruptly disappeared

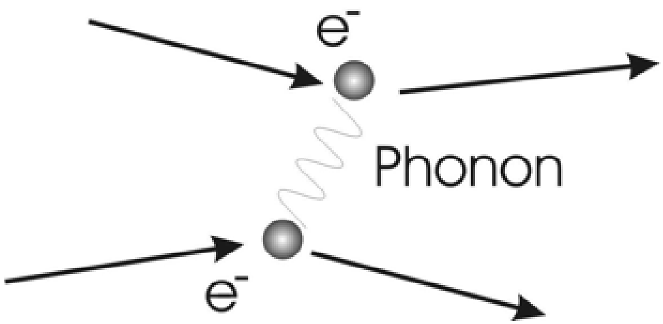
Known Superconductive Elements



Some background .....

In metals…electrical resistance is the result of electrons scattering. From translation symmetry to impurities, to lattice vibrations…

The interesting fact is…**In a superconductor material, there is a "critical temperature" where there is no "resistance"**. Electrons able to move through the lattice between positively-charged atoms/ions. A lattice distortion occurs causing a second electron to move in behind it **(Cooper pairs)**.



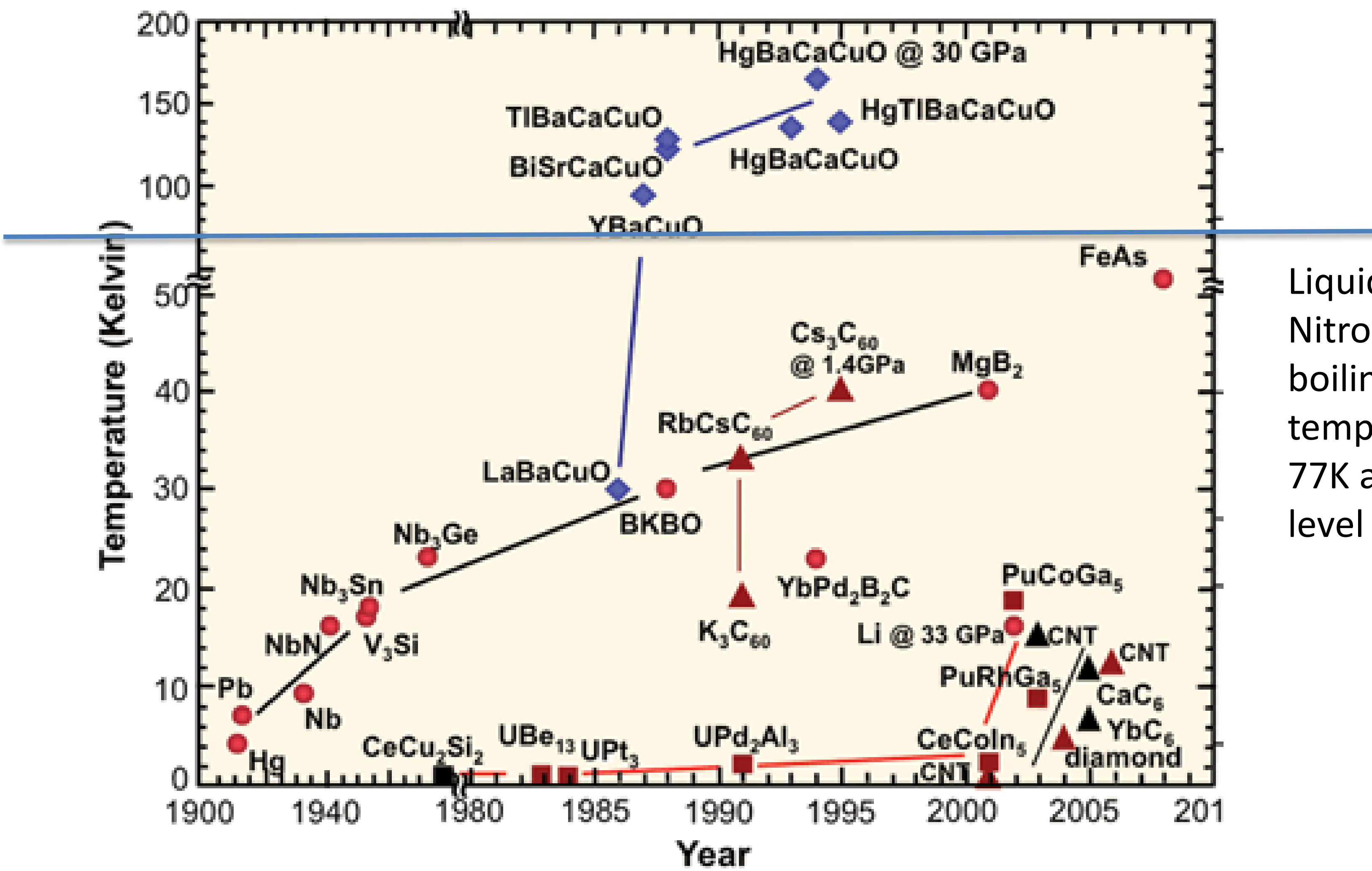
electrons coupling…depicted in a Feynman diagram

Bardeen, Cooper and Schrieffer (BCS Theory)

The two electrons form a weak attraction.
Ability to travel in a pair encountering less resistance.

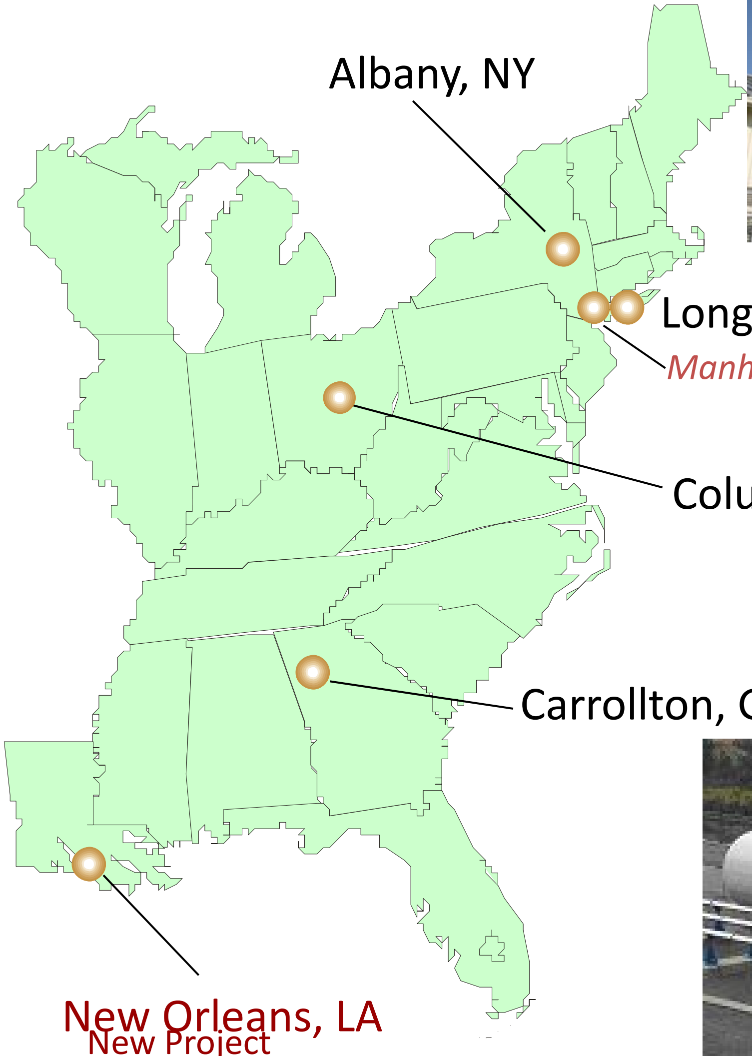
Superconductor: electron pairs (Cooper pairs) are timely forming, breaking, and forming again. The current is carried then by electrons moving in Cooper pairs (***a Quantum effect)***.

Research: Combination of Hard Work, Dedication, and Continuing Investment….*and takes time too*

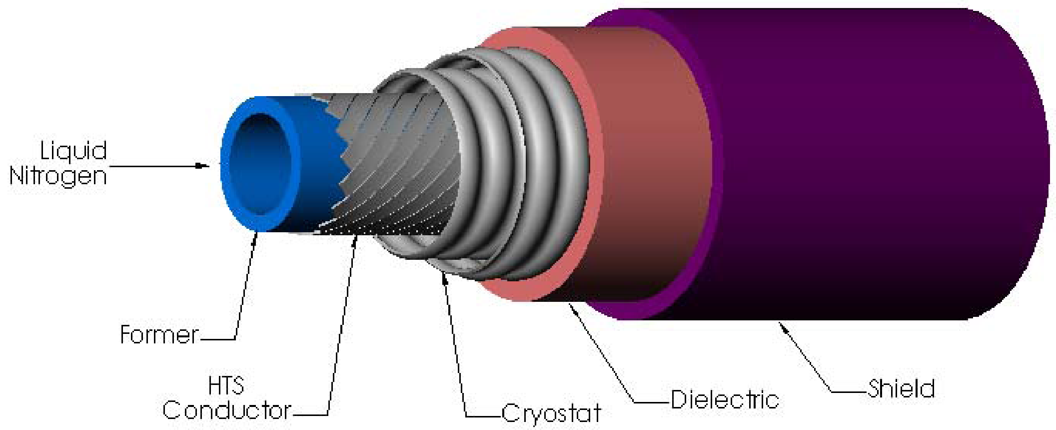


Liquid Nitrogen boiling temp. ~ 77K at sea level

U.S. HTS Cable Installations



High Temperature Superconducting Cables



Challenging and lots of opportunities:

- New Materials Research
  - From discovery
  - To functionality
  - Modeling
  - And characterization

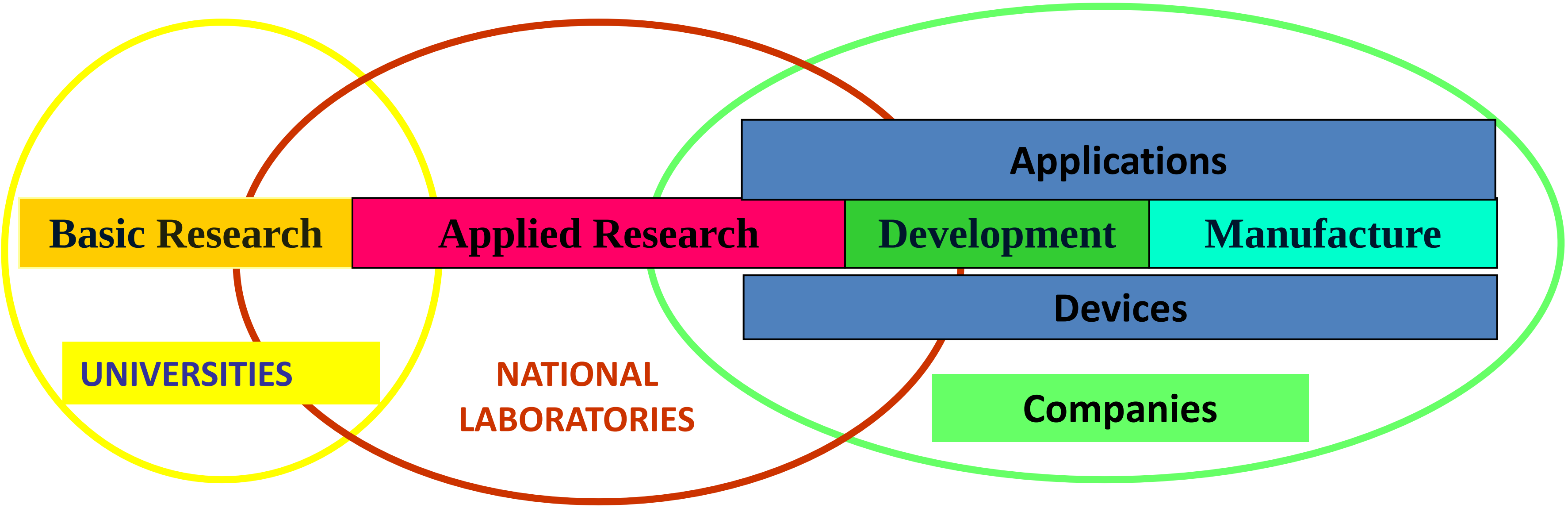
Experimental tools..

- "looking" into and designing functionality
  - Building new materials
  - The "right" tools…

However, remember....Different experimental approaches provide different views of the same "reality"

University National Labs Industry

Transferring Technology to Industry



Experimental Tools

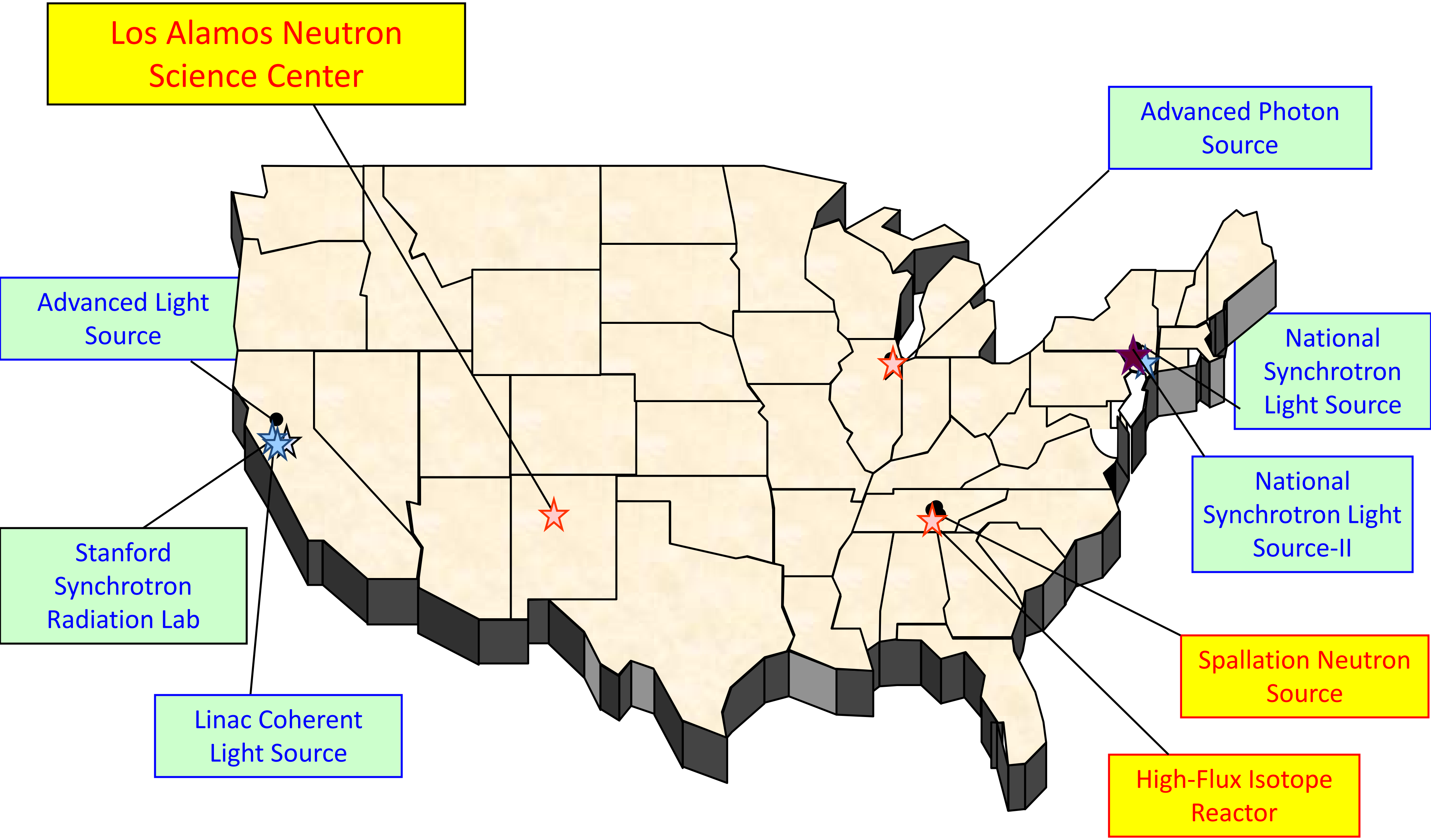
- Small/Mid: ***Universities***
- Large Scale Facilities: ***Nat. Labs***

Large Scale Experimental Facilities in the US

US Department of Energy - Office of Sciences

Light Sources & Neutrons

& Five Nano Centers User Facilities



Neutron (& Light Sources) User Facilities in EU

NEUTRONS ONLY

Asia & Australia

ANSTO (Neutrons), Australia
High-Flux Advanced Neutron Application Reactor, Korea
Japan Atomic Energy Research Institute, Japan
Japan Proton Accelerator Research Complex, Japan
Kyoto University Research Reactor Institute, Japan
Malaysia Nuclear Agency, Malaysia

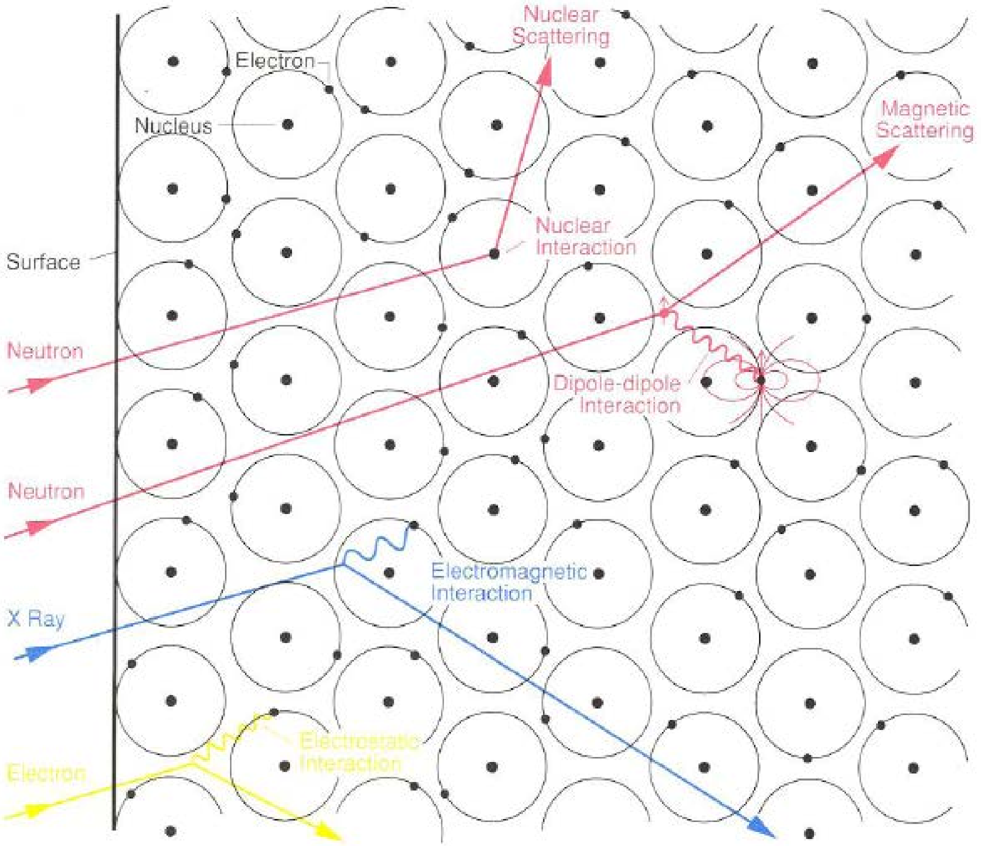
North & South America

Centro Atomico Bariloche, Argentina
Canadian Neutron Beam Center, Canada
McMaster Nuclear Reactor, Canada
Peruvian Institute of Nuclear Energy, Peru
Low Energy Neutron Source, Indiana Univ. , USA
Univ. of Missouri Research Reactor, USA
HFIR, USA
NIST, USA
SNS, USA
LANSCE, USA

Planned Facilities

Austron Spallation Neutron Source, Austria
Instituto de Pesquisas Energéticas e Nucleares, Brasil
China Advanced Research Reactor, China
China Spallation Neutron Source, China
European Spallation Source, Sweden

Interaction of Radiation with Matter



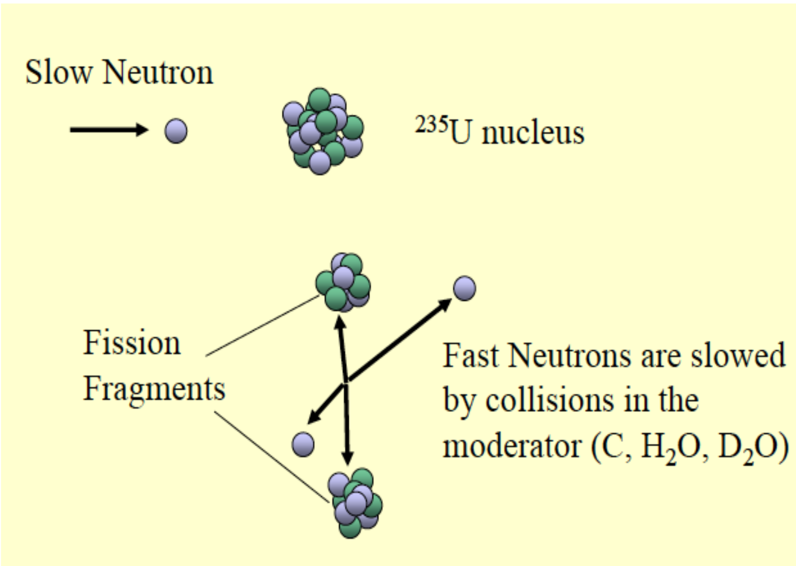
Neutron scattering as an experimental technique: Crystallography, Physics, Chemistry, Biophysics, and Materials Research in general.

Neutron experiments: Elastic scattering (diffraction) structure studies; Inelastic scattering is used for atomic vibrations and excitations in general determinations .

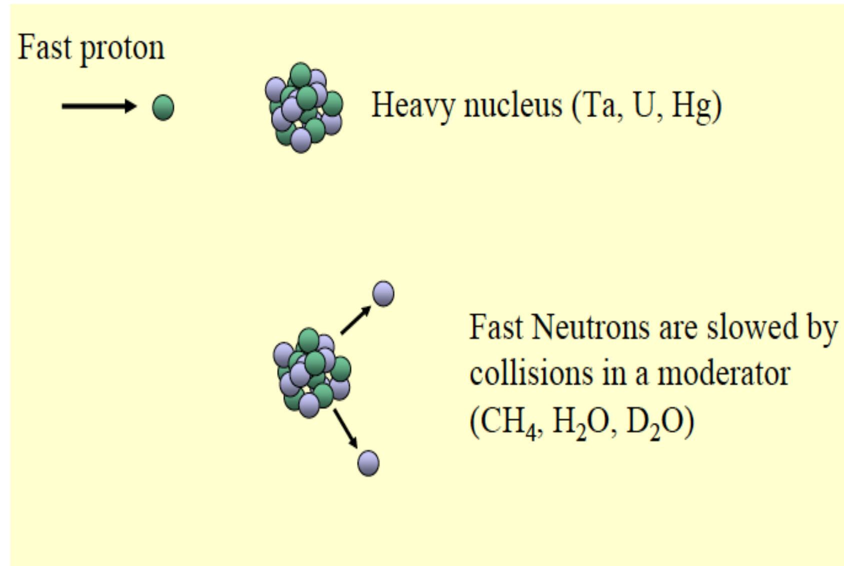
Neutrons: A modern experimental tool to understand materials properties on the atomic scale

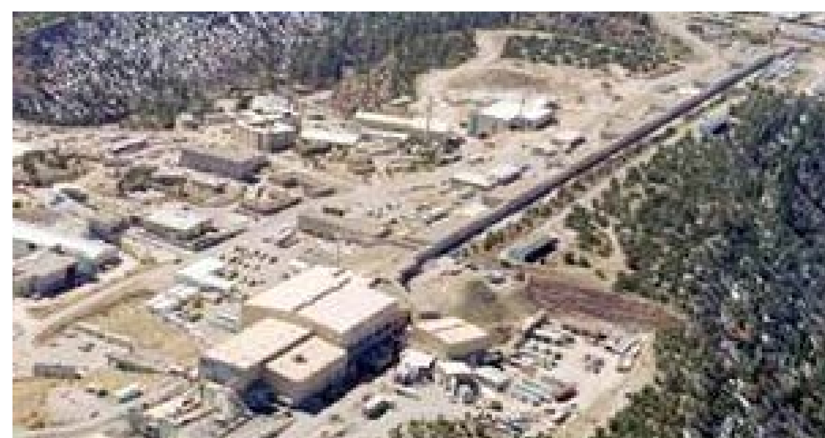
Neutron Production

Fission:



Spallation:

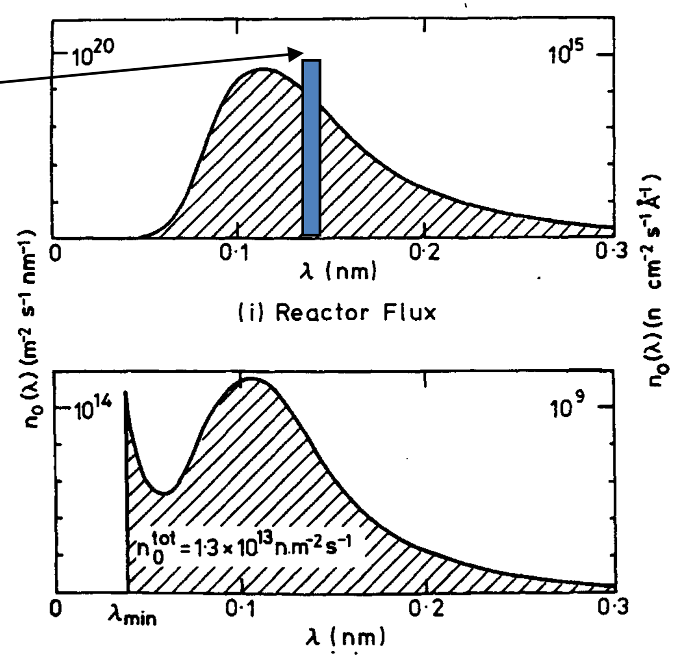




Neutron sources – steady state (Reactors) and pulsed (Spallation)

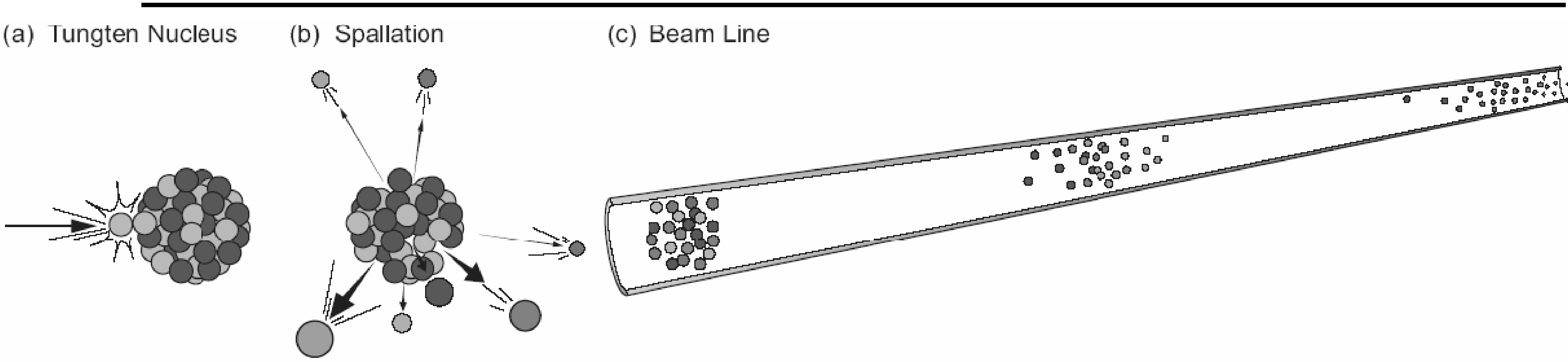
- **Reactor**
  - Fission of U^{235} produces neutrons
  - Fission spectrum moderated (slowed down) by either D_2O or H_20 (less good moderator) and neutrons are extracted through beam tubes for spectrometers – fixed wavelength used

- **Spallation**
  - High Energy protons (e.g., 800 MeV) impinge on target (W, Hg or U)
  - Nucleus of target is raised to excited state and subsequent decay produces neutrons.
  - Neutrons moderated by liquid H, H_20 or methane
  - Spallation sources generally operate in pulse mode – 20 Hz at LANSCE, 60 Hz at new SNS



Time of flight is used to sort out wavelengths

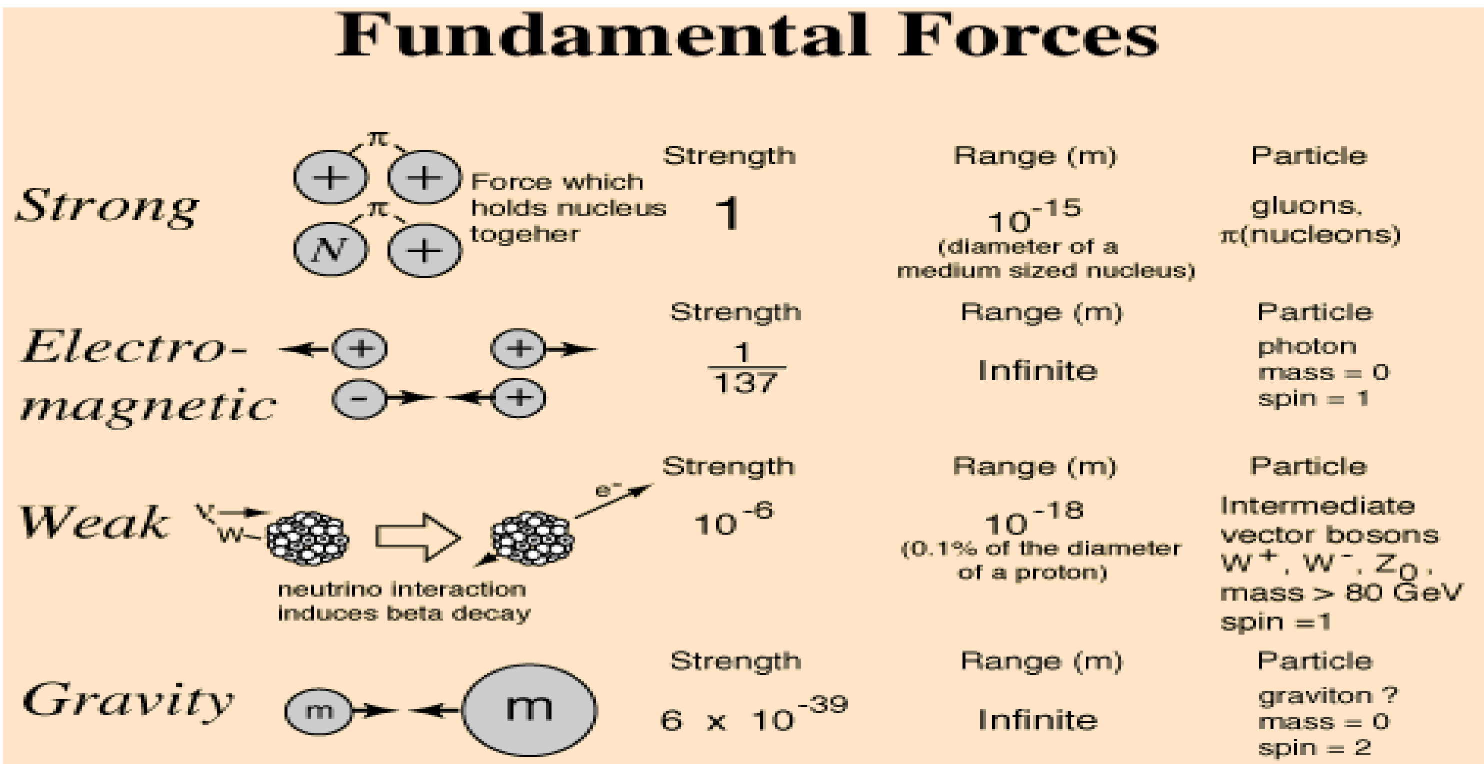
Spallation & Time-of-flight principles



- 800 MeV protons hit tungsten target
- Spallation process $\Rightarrow$ ~20 neutrons per spallation process
- Neutrons are moderated (slowed down) in H_2O
- Neutron energies between meV to 100 keV available
- Bragg diffraction: ~ 25 meV, $v \approx 3000$ m/s
- $\lambda = ht/mL \Rightarrow d = (h/2mL\sin\vartheta)\times t$
- h, m, L, $\sin\vartheta$ are constant (detectors don't move!)
- Flight paths L between 9 and 60 meter
- Constant diffractions angle simplifies design of sample environments

Why are we here: fundamental forces

Classical Mechanics (big and slow: everyday experience)	**Quantum Mechanics** (small: particles, waves)
Special relativity (fast: light, fast particles)	**Quantum field theory** (small and fast: quarks)

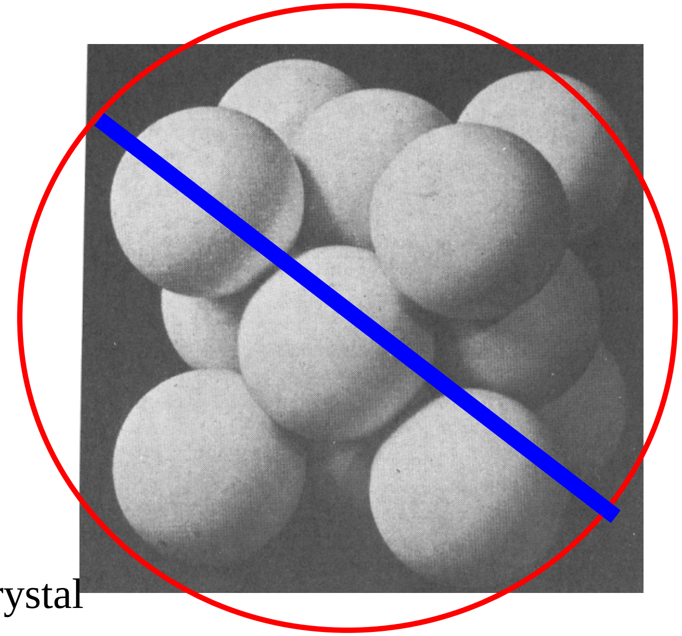


Why Use Neutrons?

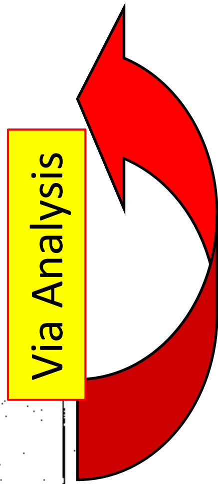
A rose in a lead container used for transporting radioactive materials. To the right is a neutron radiography image. The neutrons readily penetrate the lead container, and the hydrogen in the rose provides sufficient contrast to see even the leaves of the flower.

But, but, but….

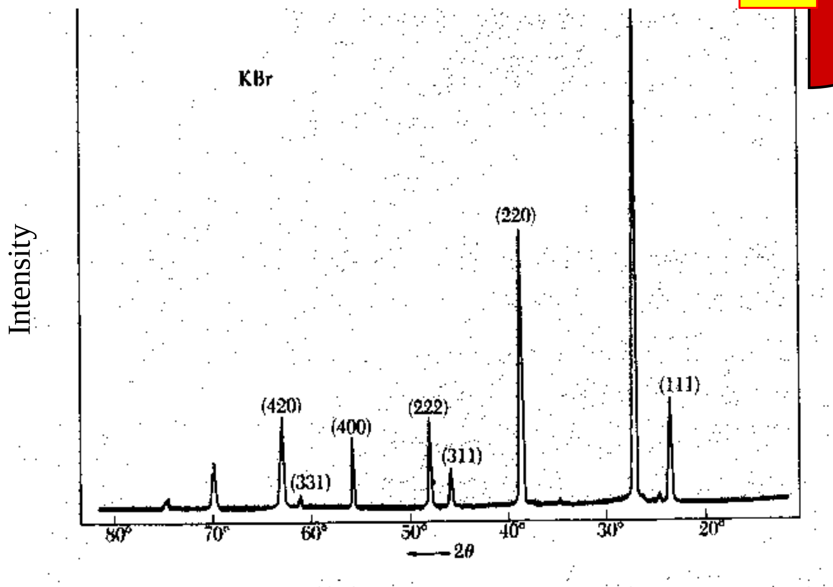
- We don’t take pictures of atoms!



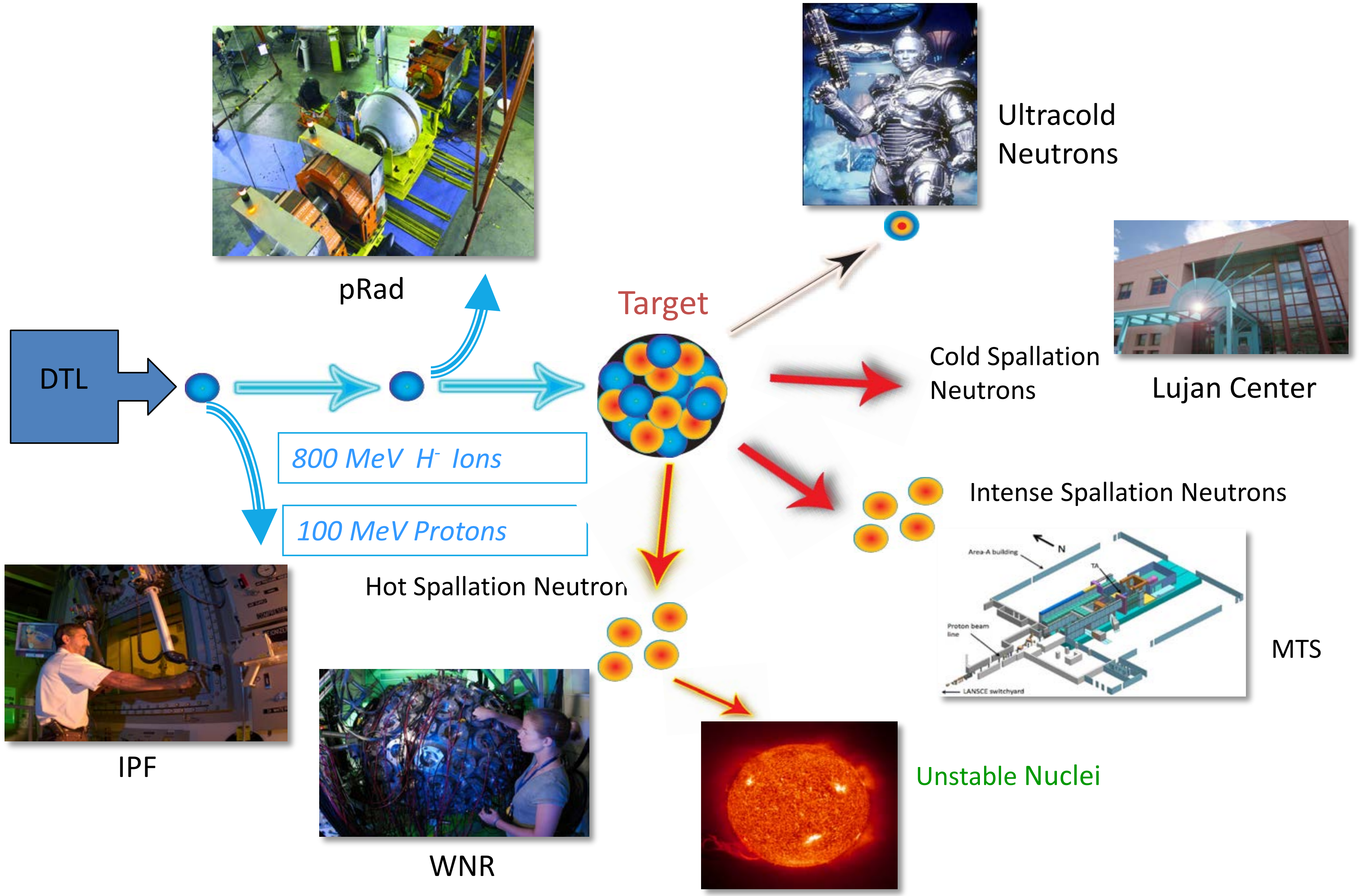
Atoms in fcc crystal



- We live in ***reciprocal space***

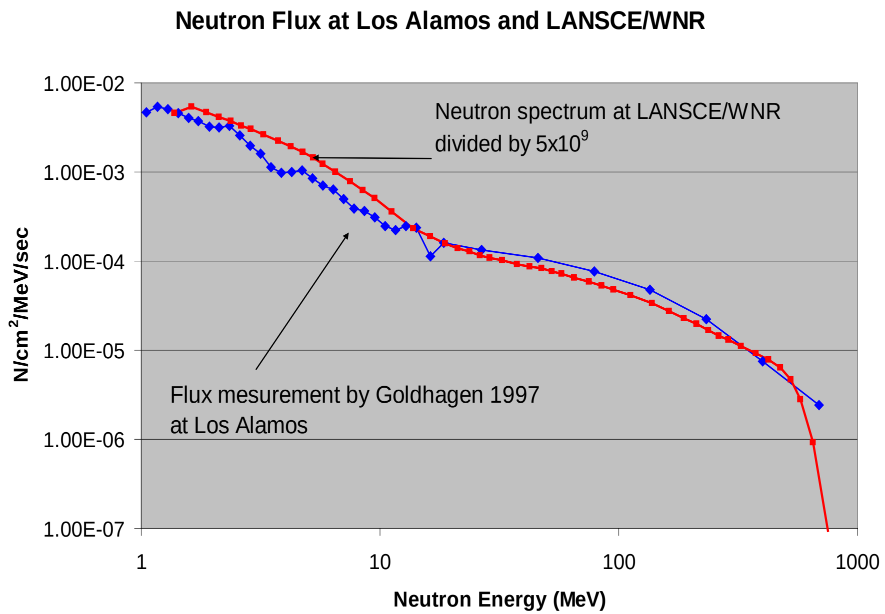


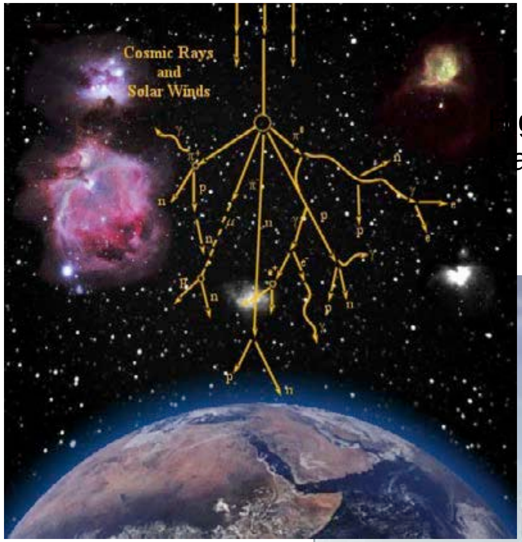
Scientists and engineers use energetic Neutrons/Protons to study matter from the subatomic to the macromolecular under normal to extreme conditions



Industrial Partnership: LANSCE SEU Beam Line

The high-energy neutron source at LANSCE provides beams of neutrons for accelerated neutron testing of semiconductors devices. Our neutron beam reproduces the naturally occurring neutron energy spectrum seen by aircraft electronics in flight, but at one million times the intensity.





gh Altitude - Atmospheric
adiation

Here

Or Here

n + Si → Si + n' + ionization trail

A Single Event Upset (SEU) is a change of state caused by ions striking a sensitive node in a micro-electronic device. Failures from neutron SEU are equal to all other failure modes combined