Neutron Scattering and Energy

Presented to the
American Conference on Neutron Scattering

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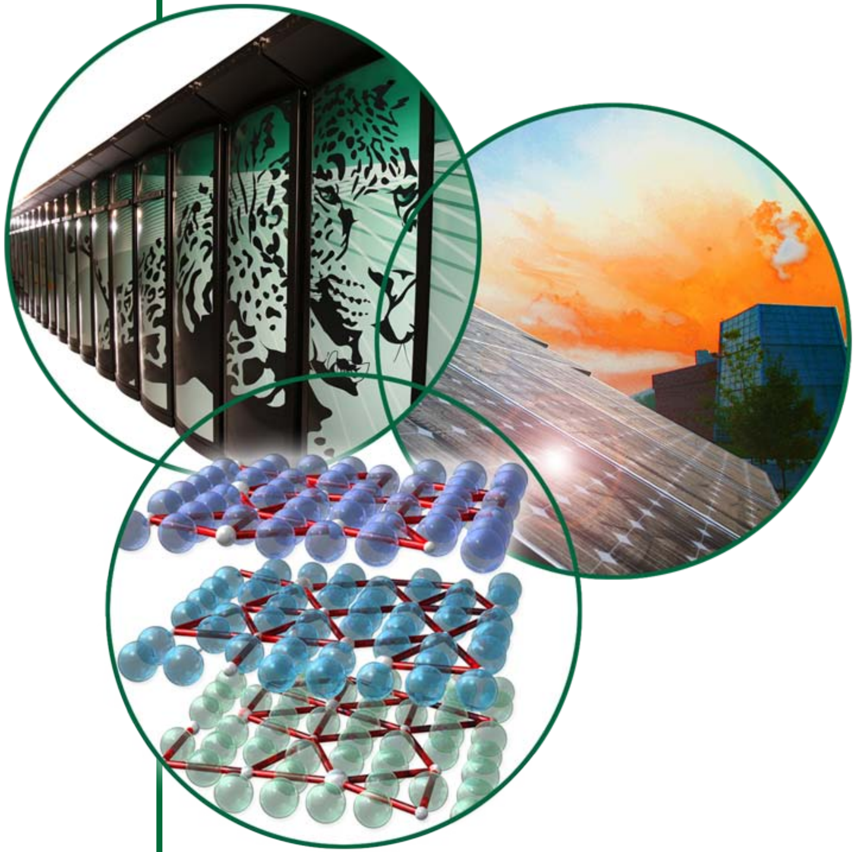
Ottawa, Ontario, Canada
June 27, 2010



U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
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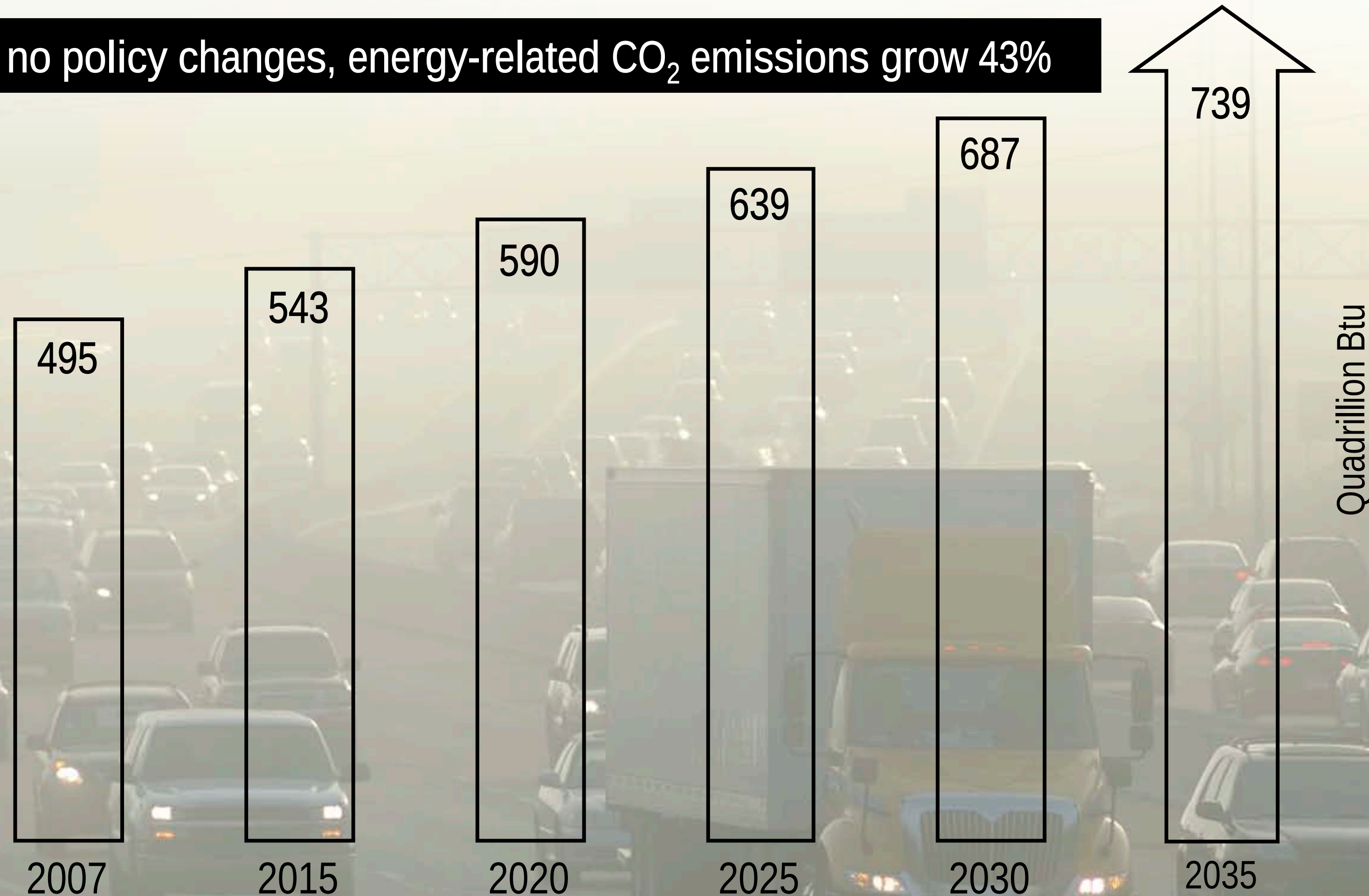
World energy consumption is projected to increase by 49% from 2007 to 2035

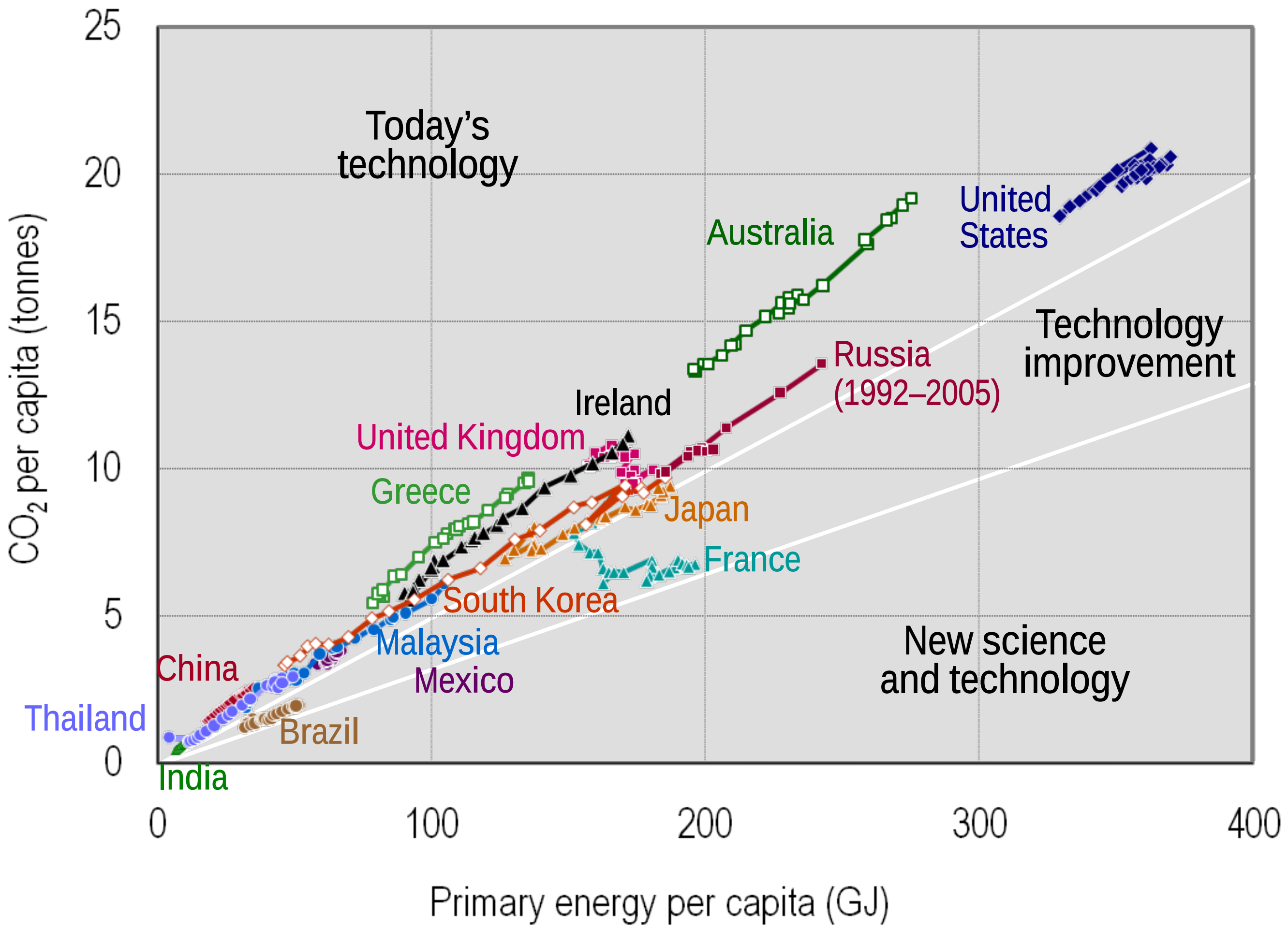
Assuming no policy changes, energy-related CO_2 emissions grow 43%



Source: Reference case, International Energy Outlook 2010, DOE/EIA-0484(2010), Energy Information Administration, May 2010

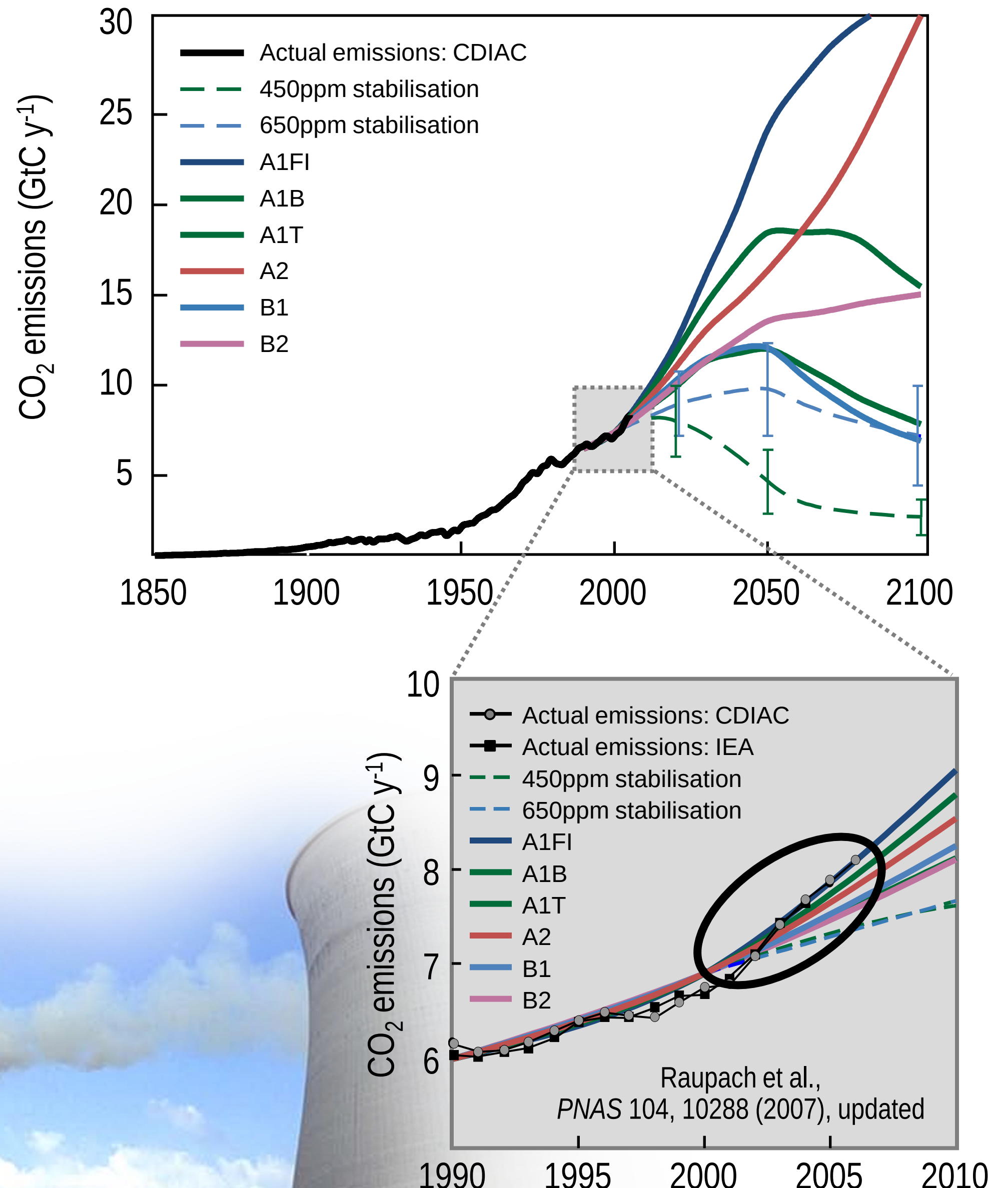
Oak Ridge National Laboratory

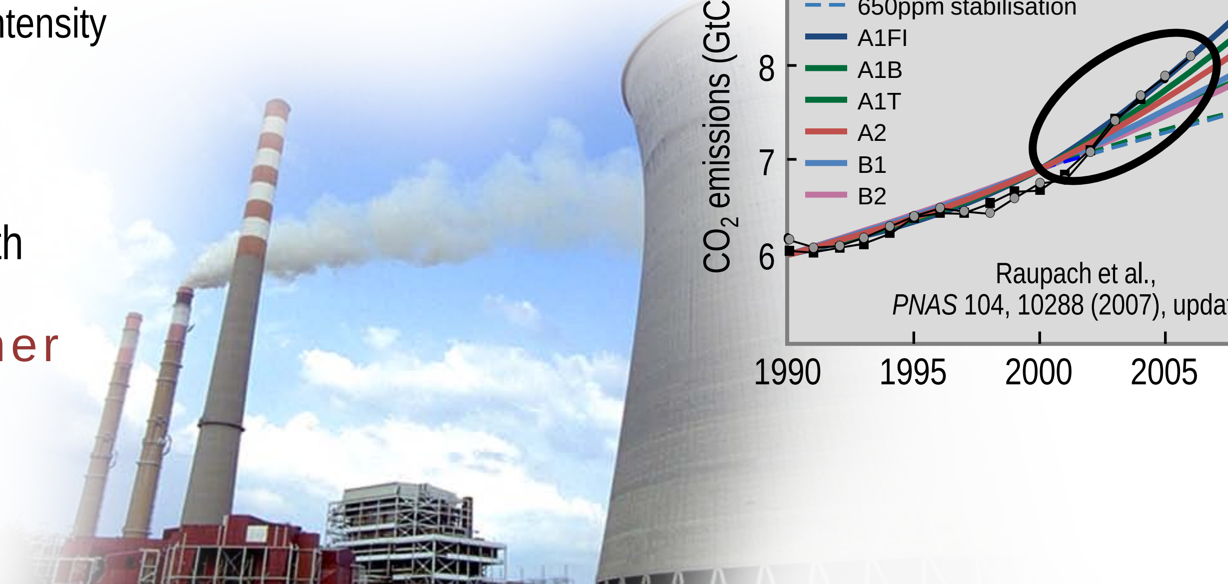
Energy use and CO_2 emissions, 1980–2005



Human activity is affecting global climate

- Atmospheric CO_2 concentrations are increasing rapidly
  - 1990–1999: +1.5 ppm per year
  - 2000–2007: +2.0 ppm per year
  - 2007: +2.17 ppm
- Three processes are contributing to this increase:
  - Growth in world economy
  - Increase in carbon intensity
  - Decline in efficiency of CO_2 sinks on land and in oceans
- Climate forcing is both **stronger** than expected and **sooner** than expected





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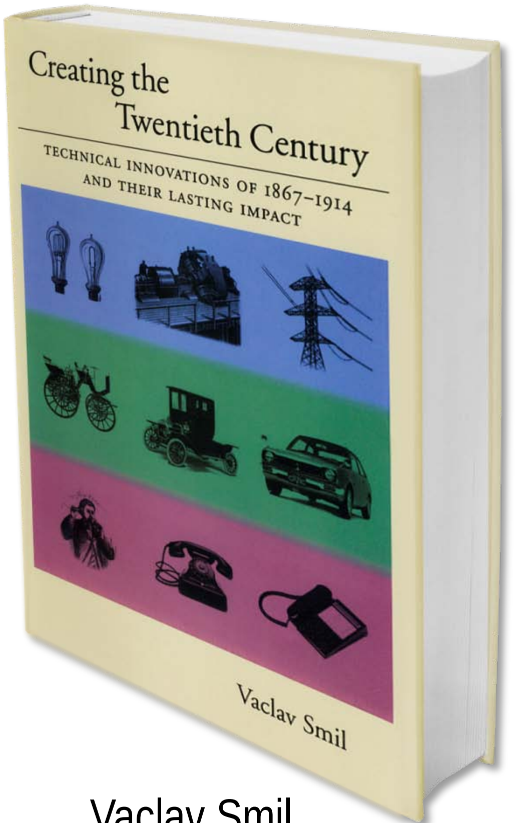
The age of synergy: 1867–1914
Phase transition in useful knowledge and its application to production

- The primary foundations for today's energy technologies and infrastructure were established before World War I
  - Electricity
  - Internal combustion engines
  - Materials and synthesis: Steel, aluminum, ammonia
  - Communication and information: Photography and radio
- With incremental improvements made throughout the 20th century, these innovations enabled the creation of the modern world
  - World population nearly quadrupled
  - World GDP increased from $1.97 trillion to $36.5 trillion



Vaclav Smil,
Oxford, 2005

Today we need another “great technical saltation”

- A new set of transformational discoveries and disruptive technologies is needed:
  - To mitigate climate change
  - To decrease our dependence on nonrenewable fossil fuels
- Leaders in innovation will drive the technology that defines the 21st century

Essential energy technologies

- Nuclear power
- Wind
- Solar
- Biofuels
- Electric drive vehicles
- Advanced liquid fuels from fossil resources

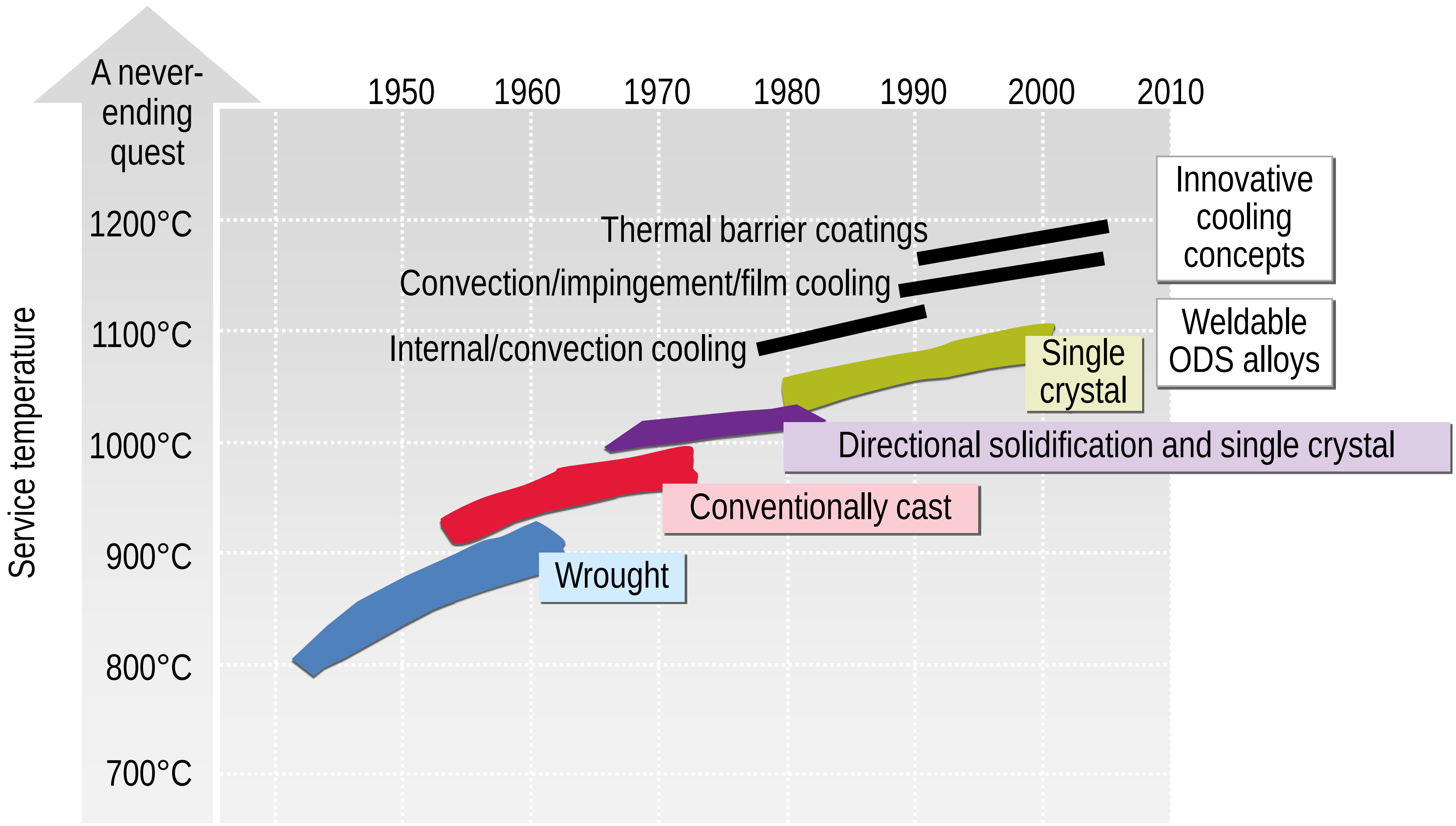
- Carbon capture and storage
- Major improvements in energy efficiency for:
  - Transportation
  - Buildings
  - Industry
  - Electricity generation and transmission

Major advances in basic science and supporting technology are needed to ensure success

The energy challenge is fundamentally a materials challenge

- Improving existing energy technologies requires increasingly robust and reliable materials
- Delivering novel capabilities requires a detailed understanding of materials structure and dynamics at the atomic and molecular level
- Understanding increasingly complex materials demands increasingly sophisticated tools

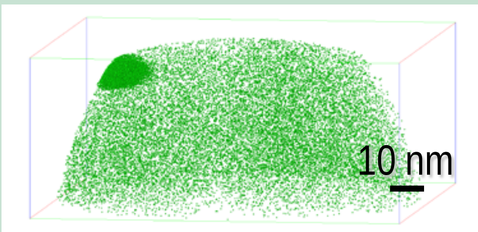
Nickel alloy development:
Higher strength and lighter weight at ever higher operating temperatures



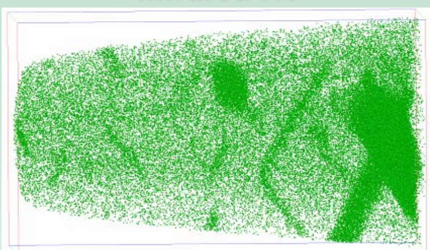
Rapid infrared heating technology for improved aluminum products

DOE-SC: BES → DOE-FE, DOE-EERE: ITP → Industry

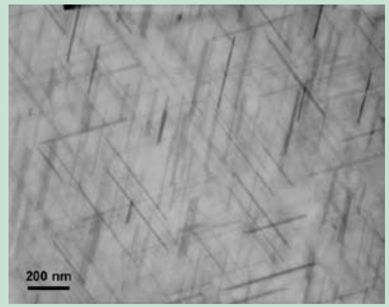
Conventional HT



Infrared HT

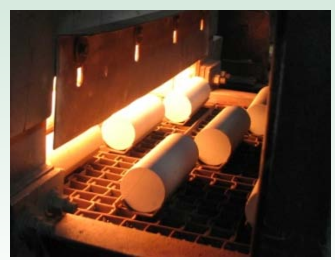


Atom probe results: Larger volume fraction of nanosize Al_2CuMg precipitates in infrared heated forgings



Research finding: Finer precipitate distribution leads to improved fatigue life

Preheating of aluminum billets

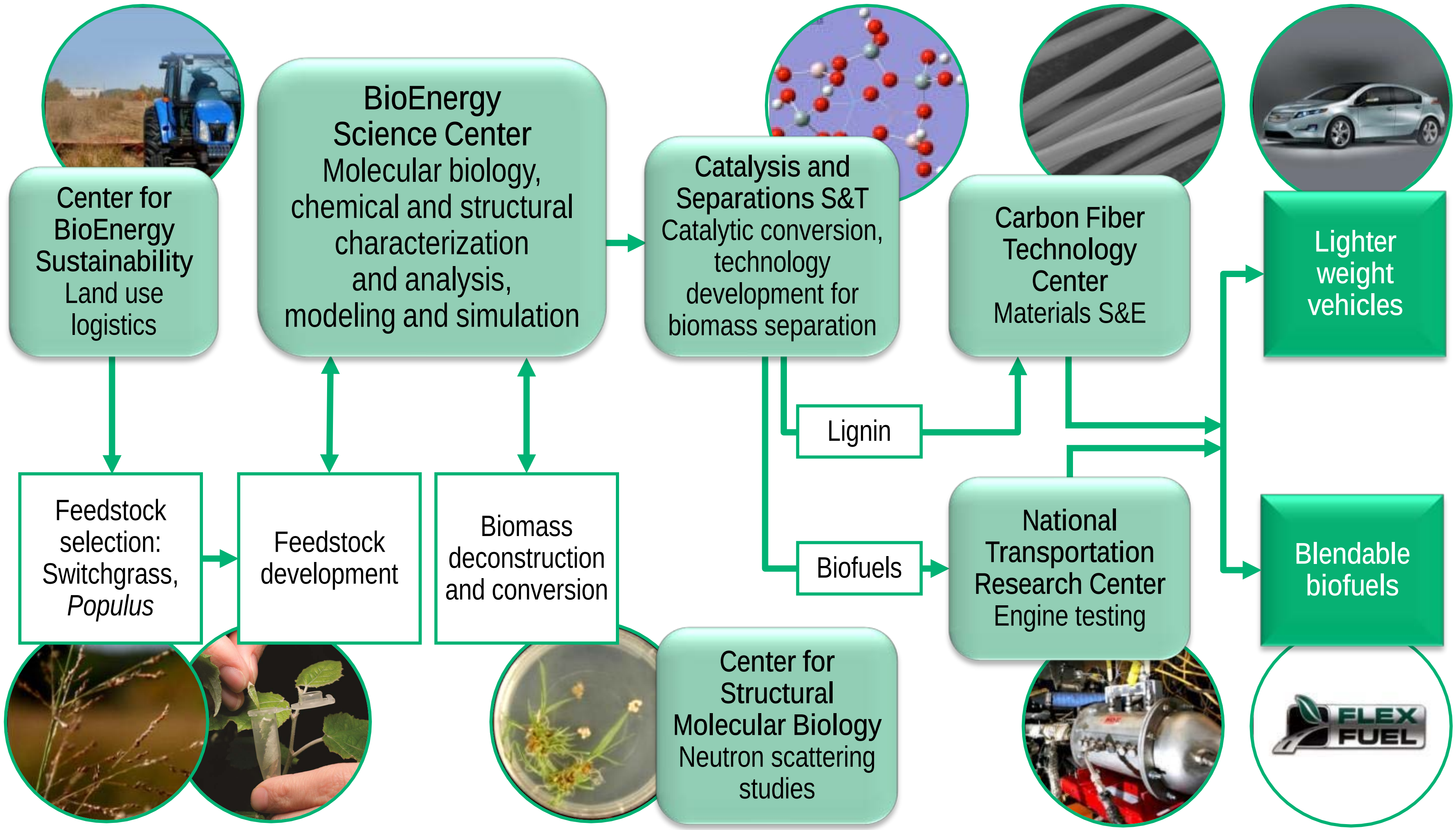


Final product: Machined impellers for diesel turbo-chargers, >300,000 parts/ year

Full-scale production: Infrared furnace operating at Queen City Forging Company, Cincinnati

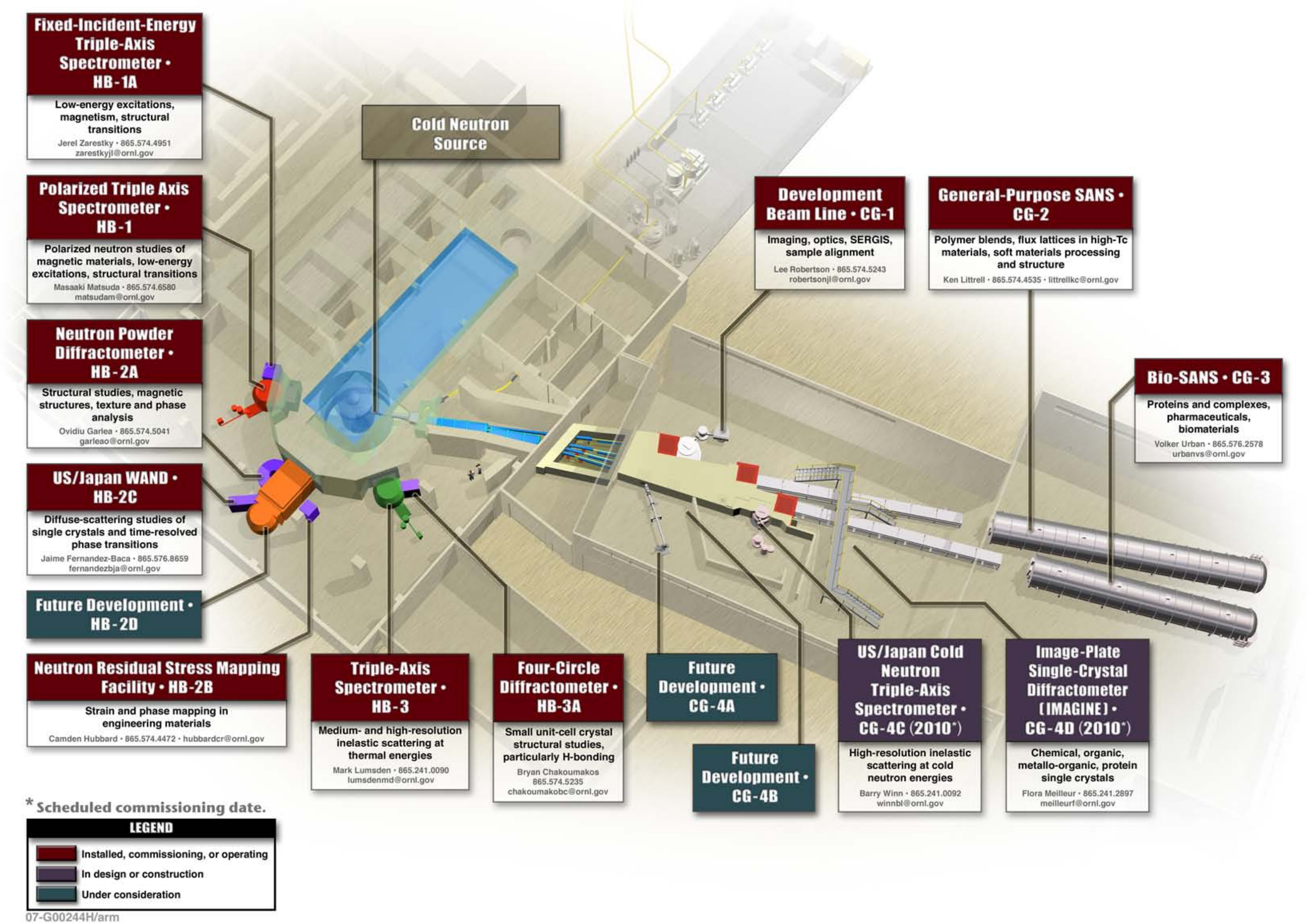
>75% more energy efficient, 3× improvement in performance, 4× improvement in production rate

Integrating science and technology for sustainable mobility

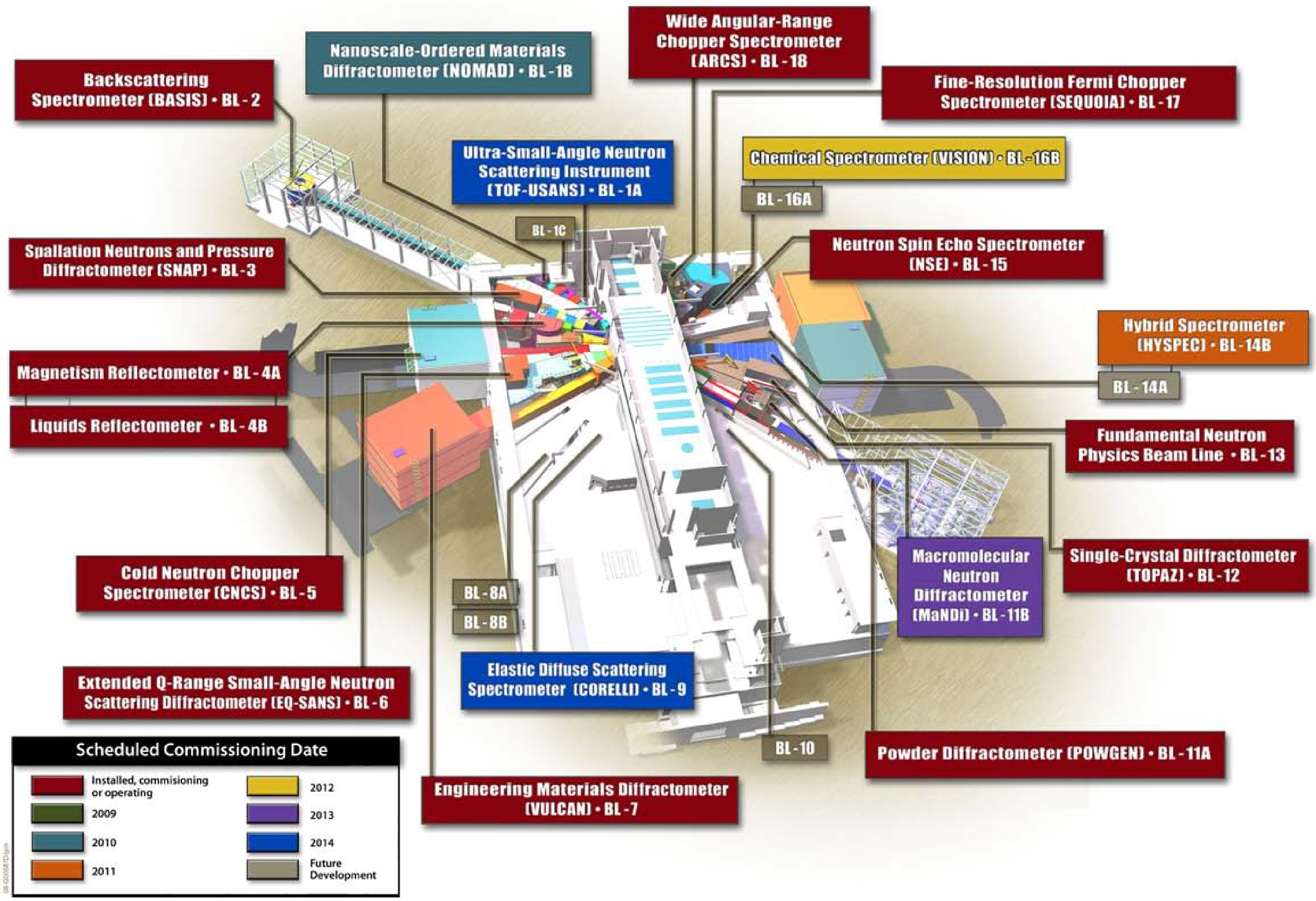


Neutrons are an indispensable tool for materials discovery and innovation

High Flux Isotope Reactor



Spallation Neutron Source



SNS upgrade plans

Science drivers

- Kinetics studies to millisecond or shorter time scales
- Dynamics of larger-scale structures (microseconds to milliseconds)
- Structures and dynamics in thin films and at interfaces
- In situ material characterization at spatial resolutions better than 10 µm

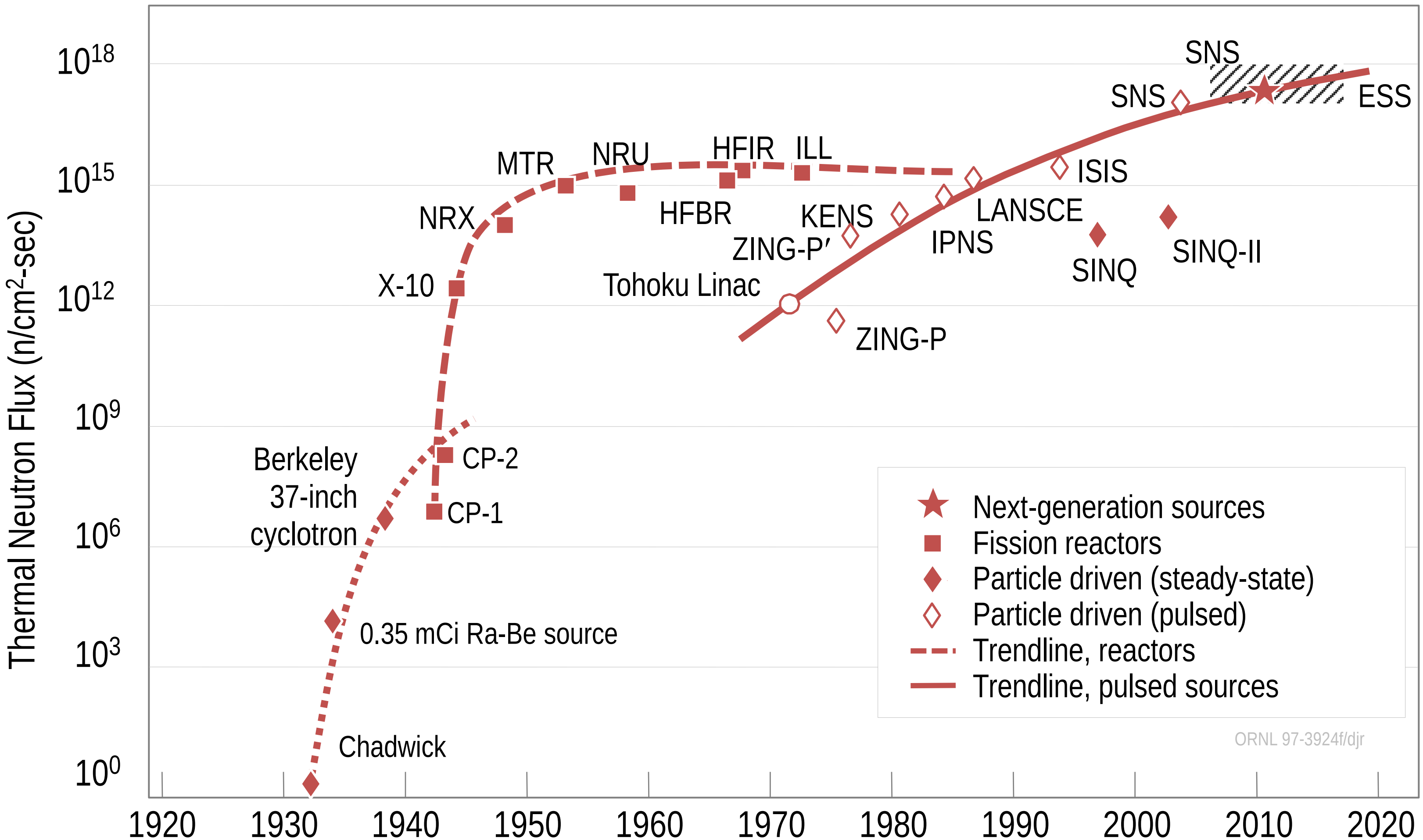
Power upgrade in progress, integrated with preparation for second target station

- CD-0 for second target station approved January 16, 2009
- Alternatives addressed for CD-1:
  - Long vs short pulse
  - Site configuration
  - Target/moderator
  - Accelerator requirements
  - Frequency
- Instrument designs show more than order of magnitude gains over first target station

Neutron scattering is providing insights for energy solutions

- High-temperature superconductors
- Environmentally friendly catalysts
- Biofuels and bioproducts from lignocellulosic biomass
- Thermoelectric materials
- Fuel cell membranes
- High-performance superalloys
- Lightweight materials for sustainable transportation
- Carbon capture and storage solutions

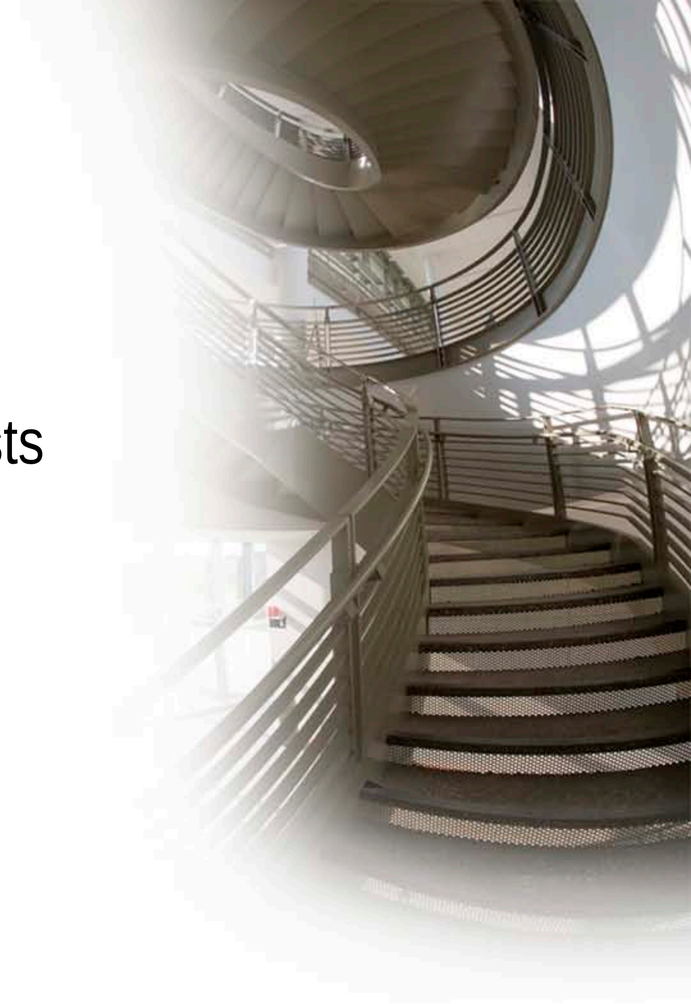
We have come a long way since 1932



(Updated from *Neutron Scattering,* K. Skold and D. L. Price: eds., Academic Press, 1986)

Continuing the journey

- Expanding the neutron user community
- Educating the next generation of neutron scientists
- Delivering the breakthroughs needed
  to enable a sustainable energy future

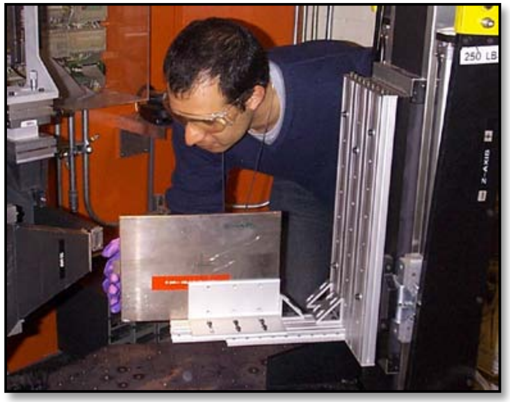


Oak Ridge National Laboratory:
Meeting the challenges of the 21st century

www.ornl.gov

Increasing energy efficiency:
Reducing the weight of heavy trucks

- Heavy-duty vehicles:
  - 4% of U.S. vehicles
  - 20% of U.S. fuel consumption
- Second Generation Neutron Residual Stress Facility (NRSF2) at HFIR: Experimental correlation of hole-cutting manufacturing processes and material choice with magnitude of residual stress and fatigue life
- Outcome: Weight of frame rails for heavy trucks can be reduced by up to 200 lb
  - Steel savings: Up to 30M lb per year
  - Fuel savings: 3.8M gal for 150,000 trucks driven 100,000 miles

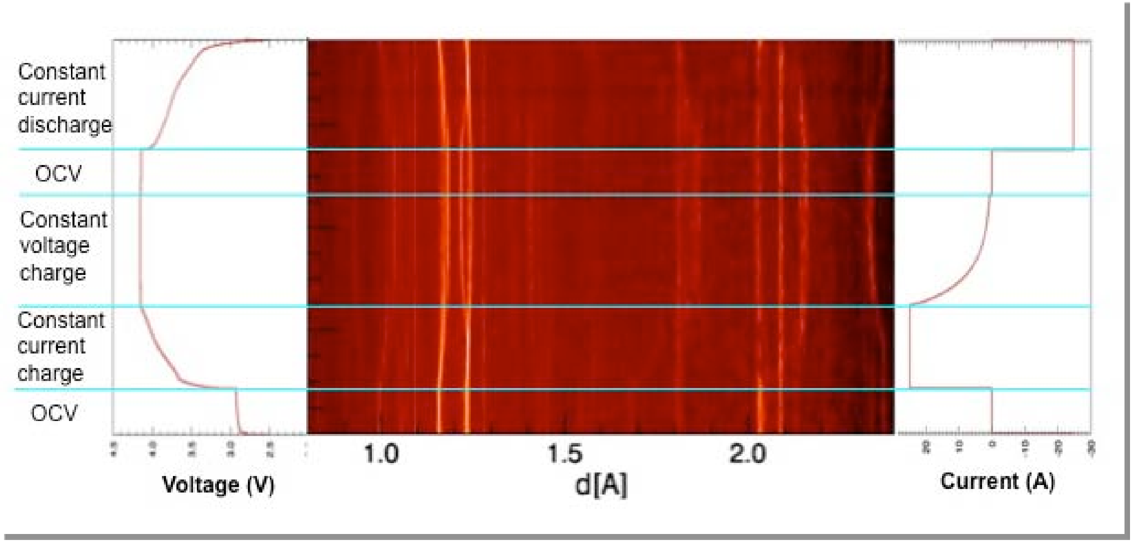


Mounting a plate test specimen for through thickness strain mapping at NRSF2

Metalsa
Quality as a way of life

Enhancing energy storage: In situ study of structure evolution during battery charge-discharge

- Investigating atomic- and nanoscale structural features in energy storage materials at SNS:
  - In situ neutron diffraction measurements
  - Event-based data acquisition
- Outcome: Knowledge applicable to design of next-generation batteries with dramatically improved capacity and long lifetime



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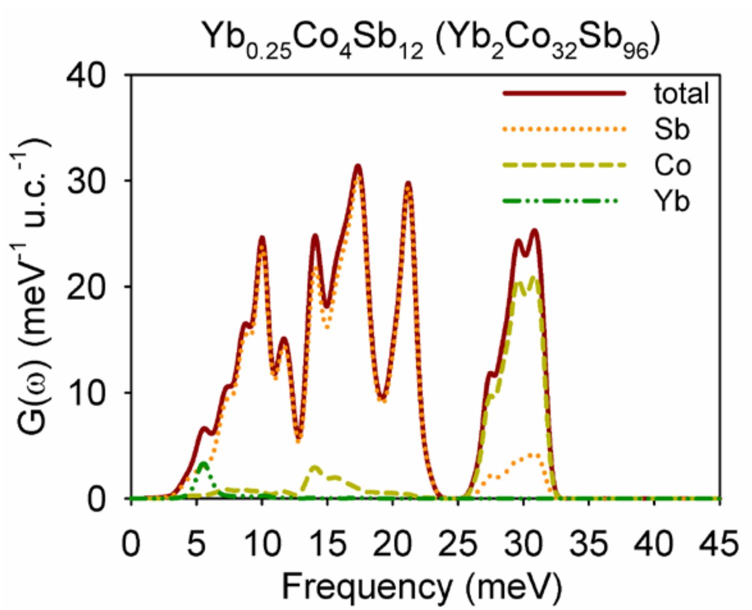
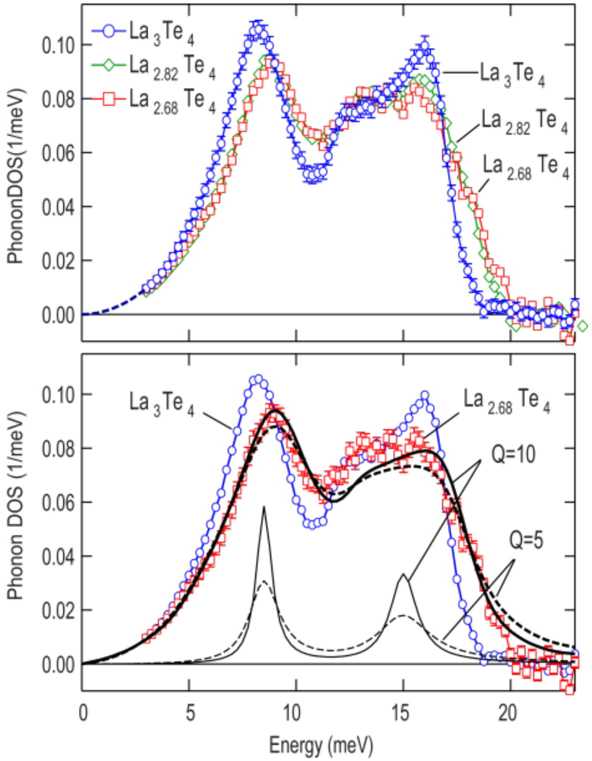
Realizing the promise of thermoelectric materials

- Cold Neutron Chopper Spectrometer at SNS: Studies of cerium- and ytterbium-filled ternary skutterudites
  - High thermoelectric figure of merit ZT
  - Promise for applications at 400–800 K



- Wide Angular-Range Chopper Spectrometer (ARCS) at SNS: Measurement of phonon density of states (DOS) in lanthanum telluride by inelastic neutron scattering



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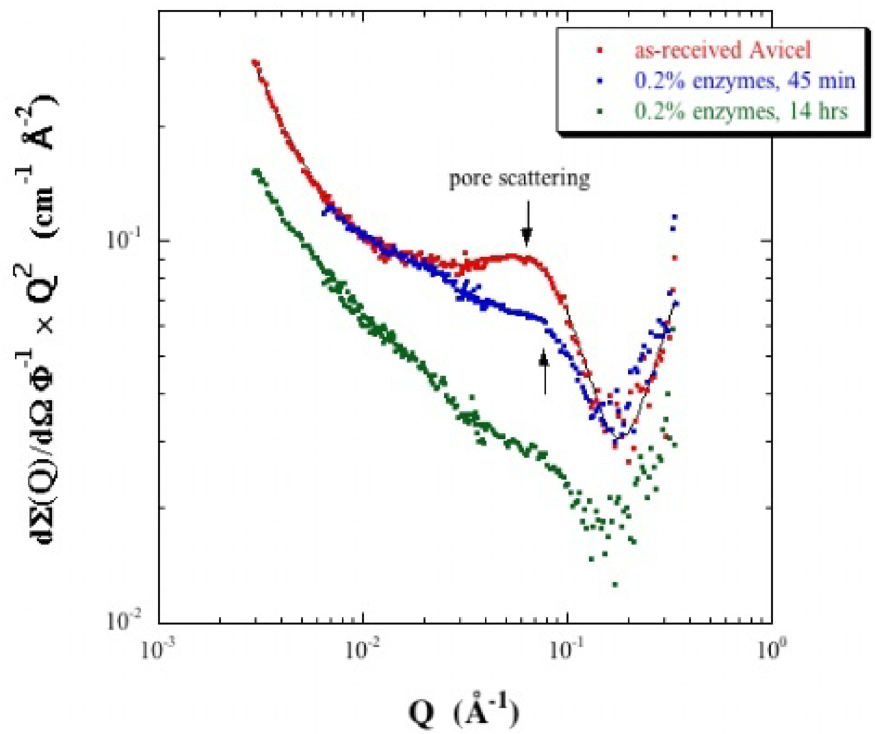
Biomass to biofuels:
Probing cellulose digestion

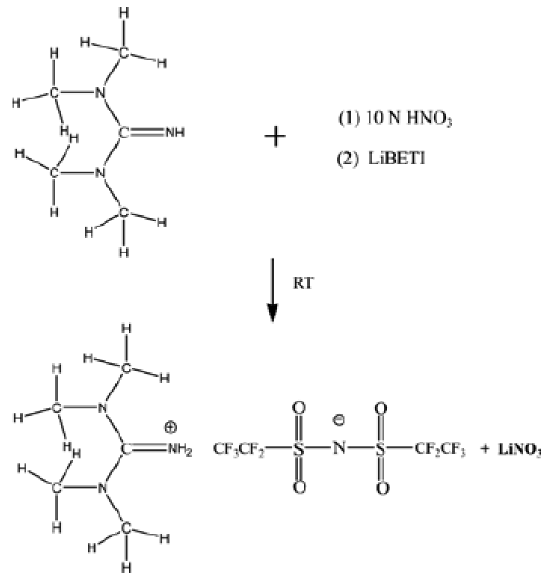
- Improving the efficiency of enzymatic digestion of cellulose biomass would reduce the cost of producing fermentable sugars
- Bio-SANS at HFIR: First neutron scattering study of the structure of Avicel (FD100) microcrystalline cellulose during enzymatic digestion
- Outcome: Significant agitation is required in order for enzyme digestion to affect nanopore structure

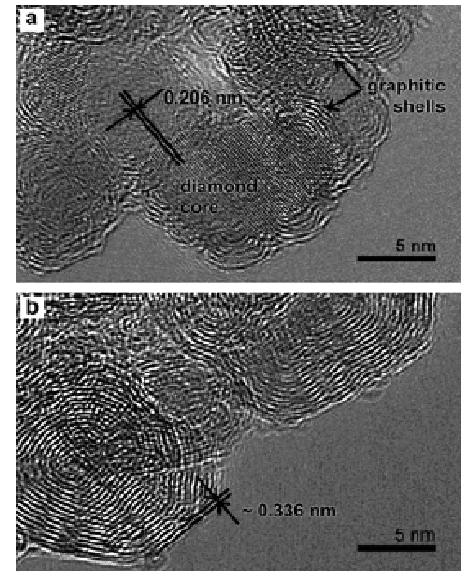


Bio-SANS data obtained during dynamic digestion: Roll-off in intensity decreases rapidly after introducing enzymes, indicating that rapid digestion occurs in or around water-filled pores

Enhancing energy storage:
Studying the mobility of ions in room-temperature ionic liquids

- Backscattering Spectrometer (BASIS) at SNS:
  QENS used to identify several distinct dynamic components in RTILs in bulk form
- Current work at ORNL Fluid Interface Reactions, Structures, and Transport Center (a DOE EFRC): Studies of RTILs confined in carbon-based nanomaterials, such as nano-onions, and other mesoporous media
- Potential for ionic charge-carrying media for advanced batteries and supercapacitors

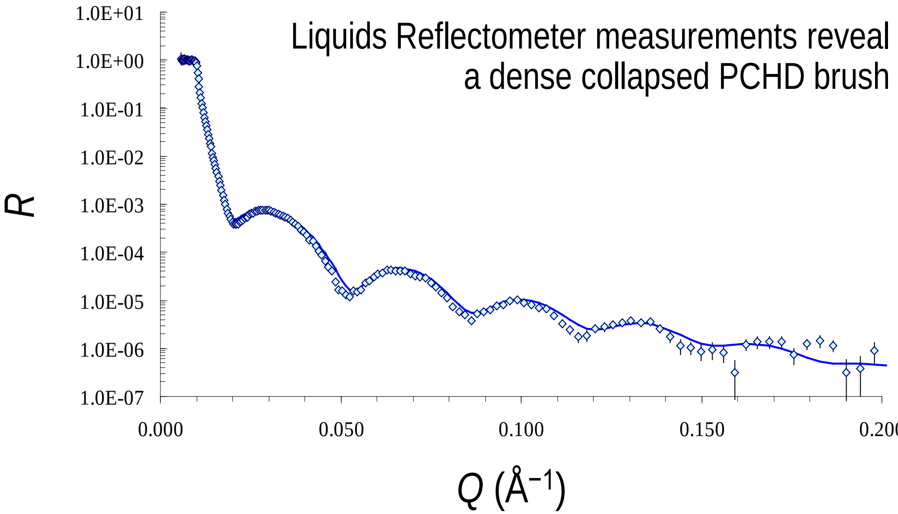




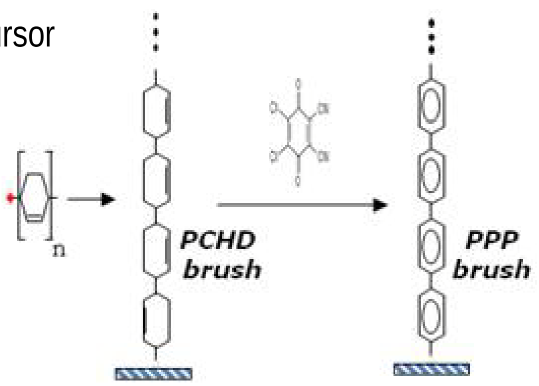
Structure of RTIL confined in carbon nano-onions

Materials for advanced energy systems: Polymer films

- Liquids Reflectometer at SNS: Studies of the internal structure of conducting polymers, aimed at understanding impact on properties of:
  - Control of regularity of structure
  - Control of morphology at the interface
- Researchers have mastered synthesis and deposition and begun characterization with neutron reflectivity and other techniques
- Potential applications: Electrical conductors for solar energy, proton conductors for fuel cell membranes

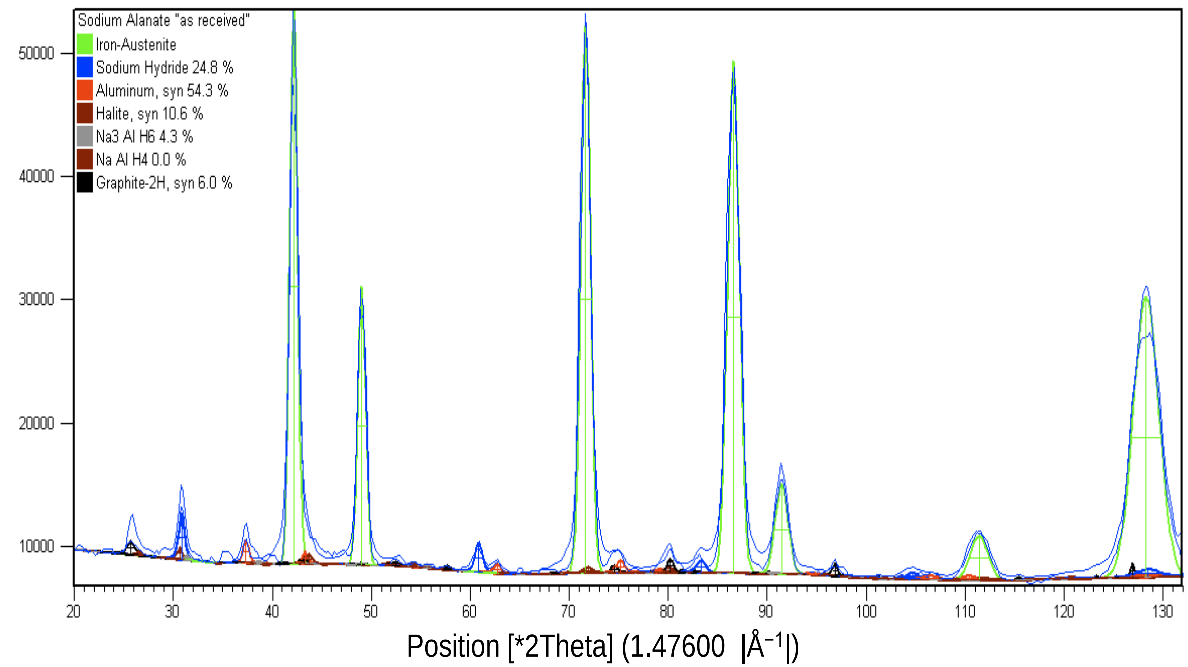


Poly(cyclohexadiene) precursor grown from Si substrate and aromatized by exposure to 2,3-dichloro-5,6-dicyano-1,4-benzoquinone to yield conducting poly(p-phenylene)



Developing hydrogen storage media

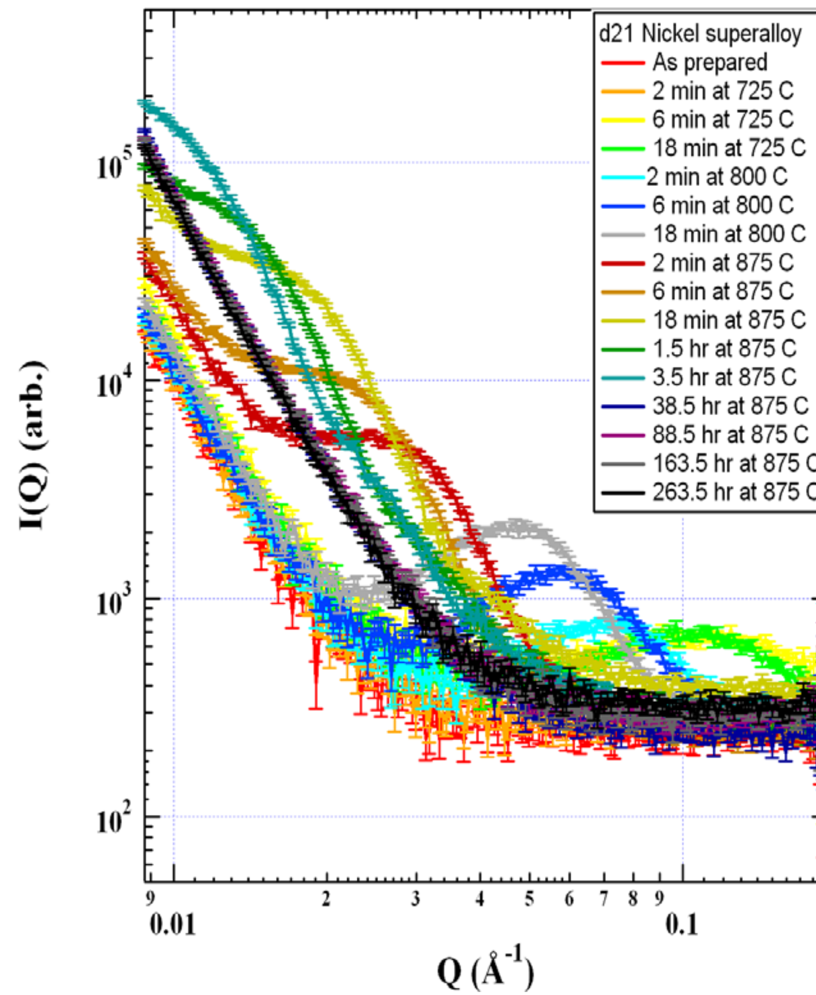
- Wide-Angle Neutron Diffractometer at HFIR: Characterization of hydrogen content in tubes charged with sodium alanates, to provide first 3D map of hydrogen absorption in specific locations and how it changes as tubes fill
- Results:
  - Resolution of C, NaH, NaCl, Na_3AlH_6, and Al phases in uncharged tube
  - Resolution of alanate peaks in discharged and partially charged tubes
- In situ absorption/ desorption experiments with deuterium to be conducted on VULCAN at SNS and neutron imaging capability at HFIR



Quantitative phase analysis of as-received powder in steel tube

Longer lifetimes for power generation equipment: Nickel-based superalloys

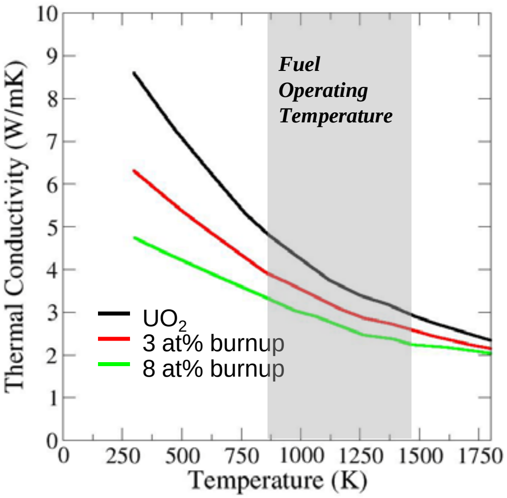
- General Purpose SANS at HFIR: Analysis of effects of repeated heating and cooling cycles on arrangement of inclusions in Waspaloy
  - Changes in precipitate distribution with repeated thermal exposure/cycling
  - Clear trends in increasing correlation distance between precipitates as a function of ex situ heat treatment
- Information on changes in electrical response with crack formation will enable development of better monitoring techniques to identify flaws before component failure
  - Longer life
  - Higher reliability

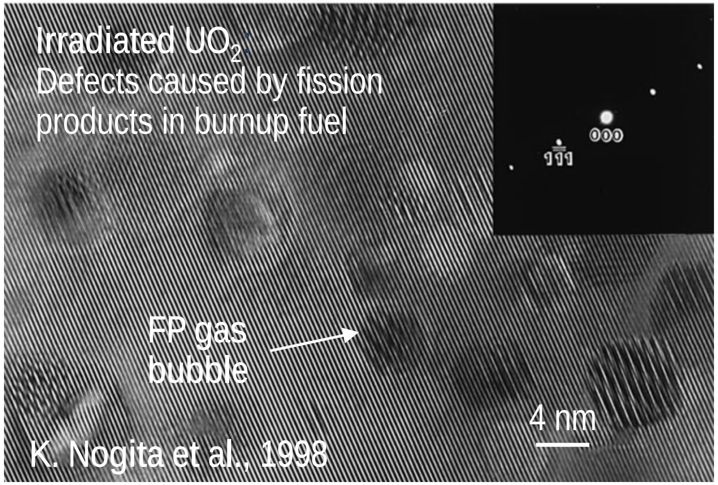


Understanding thermal transport in model nuclear fuel UO_2

- Oxide nuclear fuel:
  - Thermal conductivity is inherently low
  - Radiation effects further reduce conductivity
- SNS and HFIR: Phonon dispersion and line width/lifetime measurements will clarify impacts of
  - Temperature (anharmonicity)
  - Radiation-induced defects (e.g., fission product impurities)
  - Stoichiometry
- Experiments will test and guide simulations of thermal transport in UO_2 under temperature and lattice defects
  - Advanced MD modeling
  - Boltzmann transport equation

From Lucuta et al., 1996: Measurements using SIMFUEL (simulated high-burnup UO_2-based fuel)





Center for Materials Science of Nuclear Fuel
U.S. DEPARTMENT OF ENERGY Energy Frontier Research Center

Sustainable mobility: Biomass for biofuels and carbon fiber

Cellulose and hemicellulose

Chemical building blocks: Plastics, industrial additives, biomedical applications

Ethanol fuel

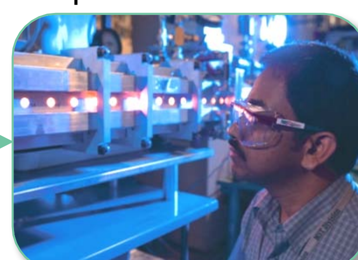
BESC
BioEnergy Science Center

Lignin

Reduction in finished carbon fiber production cost: ~30–40%

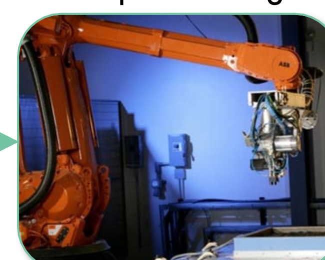
Melt spinner

Carbon fiber production line



Conversion cost: 30% of conventional

P4 preforming



Lignin and innovative processing: ~50% less than PAN and conventional processing